160th Birth Anniversary Celebration of Acharya P. C. Ray

International Seminar on

Recent Advances in Chemistry and Material Science (RACMS-2021)

(YSC-2021)

 → Student Science Meet

(SSM-2021)



(01-03, & 07-08 **AUGUST**, 2021)

1st August, 2021 **Students' Competition** (From Class V to XII & **UG, PG Students**)

> 2nd-3rd August, 2021 **International Seminar RACMS-2021**

7th-8th August, 2021 **YSC-2021**

Organized by : Indian Chemical Society



www.indianchemicalsociety.com

Kolkata

M programics4@gmail.com

PROCEEDINGS OF THE International Seminar on Recent Advances in Chemistry and Material Sciences (2021), Young Scientist Conclave (2021) & Student Science Meet (2021)

The 160th Birth Anniversary Celebration of Acharya Prafulla Chandra Ray

01-03 & 07-08 August, 2021



Organised by

The Indian Chemical Society 92, Acharya Prafulla Chandra Road Kolkata-700 009

FOREWORD

"International Seminar on Recent Advances in Chemistry and Material Sciences (2021), Young Scientist Conclave (2021) & Student Science Meet (2021)" is being organized by the Indian Chemical Society to commemorate the 160th Birth Anniversary of Acharya Prafulla Chandra Ray, the doyen of Chemical Sciences in India. This is 16th in the series of Symposium, the first one was held in 2006, as a part of Birth day celebration of Acharya Prafulla Chandra Ray, founder President of the Indian Chemical Society.

The Indian Chemical Society, one of the oldest learned bodies of our national pride was established on May 09, 1924. Acharya P. C. Ray, after returning from Edinburgh first joined the Presidency College, Kolkata in 1889 and later in 1916, joined the Department of Chemistry, newly formed University College of Science, University of Calcutta as the Palit Professor of Chemistry. Acharya Ray was intimately associated with the Indian Chemical Society till the last breath. The school of modern chemical research established by Acharya Ray in the University College of Science, where he used to live in the later part of his life, subsequently spread over the entire country through his many illustrious disciples. Acharya Ray had always strongly advocated for effective interactions between industries and academia. He himself was the founder of Bengal Chemical and Pharmaceutical Works Ltd.

Acharya Prafulla Chandra Ray was born on August 02, 1861. The Indian Chemical Society solemnly observes this auspicious day every year in a befitting manner. This year we are going to observe the 160th Birth Anniversary of Acharya Ray by organizing a weeklong program consisting of students' competition on "Chemistry for Better Tomorrow" amongst students of Class V-XII and Science & Engineering students of UG & PG courses on 1st August. There are eighteen speakers of different research areas from theoretical to applied research in "International Seminar on Recent Advances in Chemistry and Material Sciences (2021)" to be held on 02-03 August. On 07-08 August in the "Young Scientist Conclave (2021)" twenty-two young speakers from different institutes will present their research.

In organizing the Seminar, we have received sincere co-operation from every corner, particularly the fellows/members, and many organizations for their active participation. We are thankful to all of them. We are also thankful to the Endowment and Invited speakers whose deliberations, we hope, will certainly elevate the academic standard of the Seminar to a new height, and to all the distinguished chemists and the participants who responded to our appeal spontaneously in making the Seminar a grand success. Despite our best efforts there might be some lapses, for which I sincerely tender my apology.

Professor Chittaranjan Sinha

Convener of the Symposium & Honorary Secretary, Indian Chemical Society iv

International Seminar on Recent Advances in Chemistry and Material Sciences (2021), Young Scientist Conclave (2021) & Student Science Meet (2021)

The 160th Birth Anniversary Celebration of Acharya Prafulla Chandra Ray

Advisory Committee (2021)

Professor G. D. Yadav Professor R. D. Kaushik **Professor E. Sukumar Professor Chittaranjan Sinha Professor Sudip Kumar Das** Professor A. C. Bhasikuttan **Professor Samaresh Bhattacharya** Professor Chhanda Mukhopadhyay Professor Suresh C. Ameta Professor Dulal C. Mukherjee Professor (Dr.) D. Banerjea Professor Jai P. Mittal Professor K. B. Pandeva **Professor Ramesh Chandra Professor Sunil Kumar Talapatra Professor Girjesh Govil** Professor M. C. Chattopadhyaya Professor R. N. Prasad **Professor Samir Biswas** Professor Ch. Venkata Ramana Reddy **Professor Sheo Satya Prakash** Professor Mahendra Nath Roy Professor Raniit K. Verma **Professor Anand S. Aswar** Professor Ashok Kumar Mallik **Professor Homendra Naorem** Professor P. K. Dutta Professor A. Ghosh Professor Surajit Chattopadhyay **Professor Pranab Ghosh** Professor B. K. Das Professor A. D. Sawant Dr. Ramakumar Dr. Sanjeev Katti Dr. Anjan Ray

President Vice President Vice President Honorary Secretary Honorary Treasurer Honorary Editor Honorary Editor Honorary Editor Advisor **Council Member** Council Member **Council Member** Council Member Council Member Council Member Council Member Manipur University, Imphal Allahabad, Uttar Pradesh VC, Rani Rashmoni Green University, West Bengal Kalyani, West Bengal North-Bengal University, Darjeeling Guwahati, Assam Editor IOC, Council Member (Industry) ONGC, Council Member (Industry) Director, CSIR-IIP

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International Seminar on Recent Advances in Chemistry and Material Sciences (2021), Young Scientist Conclave (2021) & Student Science Meet (2021)

The 160th Birth Anniversary Celebration of Acharya Prafulla Chandra Ray

PROGRAMME

1st August, 2021

10.00-10.30 am: Welcome to the competitors & judges Students' Competition (From Class V to XII & UG, PG Students) (10.30 am-2.30 pm) (IST)

Group – A:

Class V – VI

Topic: Our Environment, Our life

Group – B:

Class VII - VIII

Topic: Sustainable development: Future Agroindustry

Group – C:

Class IX – X

Topic: Crisis and conservation of Water

Group – D:

Class XI – XII

Topic: Energy Sustainability

Group – E:

UG Students of Science & Technology Departments

Topic: Corona Virus: Prevention and possible remedial measures

Group – F:

PG Students of Science & Technology Departments

Topic: Corona Virus: Prevention and possible remedial measures

Seminar-1 (Day-1) 2nd August 2021 (10.00 am-06.00 pm) (IST) Session-I (10.00 am-12.00 pm) (IST)

9.30-9.40 am	:	Garlanding to Acharya P. C. Ray in Head Quarter
9.40-10.00 am	:	Introduction by Prof. D. C. Mukherjee, Advisor, ICS
10.00-10.30 am	:	Inaugural Address by Prof. G. D. Yadav, President of ICS
10.30-10.35 am	:	Felicitation of Lifetime Achievement Awardee, Prof. J. S. Yadav
10.35-11.05 am	:	Keynote Address by Prof. J. S. Yadav
11.05-11.35 am	:	Acharya Prafulla Chandra Ray Memorial Endowment Award
		Lecture (2019) by Prof. Samaresh Bhattacharya, Jadavpur University
11.35-11.45 am	:	Address by Prof. Chittaranjan Sinha, Honorary Secretary, ICS
11.45-11.50 am	:	Vote of thanks by Prof. Sudip K. Das, Honorary Treasurer, ICS

Session-II Invited Lectures (12.00 pm-1.30 pm) (IST)

Chairperson: Prof. Ethirajan Sukumar drsuku3@gmail.com

12.00 pm-12.30 pm :		Invited Lecture 1			
		Speaker	:	Dr. Rajendra Joshi	
				RI Nanotech India, Uttarakhand	
				rjoshinano@gmail.com	
12.30 pm-1.00pm	:	Invited Le	ctur	e 2	
		Speaker	:	Prof. Alakesh Bisai	
				IISER Kolkata	
				alakesh@iiserkol.ac.in	
1.00 pm-1.30 pm	:	Invited Le	ctur	e 3	
		Speaker	:	Dr. S. S. V. Ramakumar	
				IOCL, Faridabad	
				ramakumarssv@indianoil.in	
1.30 pm-2.00 pm:	Lu	unch Break			

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Session-III Invited Lectures (2.00 pm-5.00 pm) (IST)

Chairperson: Prof. Samaresh Bhattacharya samaresh_b@hotmail.com

2.00 pm-2.30 pm	:	Invited Lecture 4	
		Speaker :	Prof. Chandan Mukherjee
			IIT Guwahati, Assam
			cmukherjee@iitg.ac.in
2.30 pm-3.00 pm	:	Invited Lectur	e 5
		Speaker :	Prof. Deepak Chopra
			IISER Bhopal
			dchopra@iiserb.ac.in
3.00 pm-3.30 pm	:	Invited Lectur	e 6
		Speaker :	Dr. Kamalika Sen
			University of Calcutta, Kolkata
			kamalchem.roy@gmail.com
		Chairp	person: Prof. R. N. Prasad
			rnp_1949@yahoo.co.in
3.30 pm-4.00 pm	:	Invited Lectur	rnp_1949@yahoo.co.in e 7
3.30 pm-4.00 pm	:	Invited Lectur Speaker :	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal
3.30 pm-4.00 pm	:	Invited Lectur Speaker :	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar
3.30 pm-4.00 pm	:	Invited Lectur Speaker :	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar dmandal@iitrpr.ac.in
3.30 pm-4.00 pm 4.00 pm-4.30 pm	:	Invited Lectur Speaker : Invited Lectur	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar dmandal@iitrpr.ac.in e 8
3.30 pm-4.00 pm 4.00 pm-4.30 pm	:	Invited Lectur Speaker : Invited Lectur Speaker :	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar dmandal@iitrpr.ac.in e 8 Prof. Guo Zhanhu
3.30 pm-4.00 pm 4.00 pm-4.30 pm	:	Invited Lectur Speaker : Invited Lectur Speaker :	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar dmandal@iitrpr.ac.in e 8 Prof. Guo Zhanhu University of Tennessee Knoxville, USA
3.30 pm-4.00 pm 4.00 pm-4.30 pm	:	Invited Lectur Speaker : Invited Lectur Speaker :	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar dmandal@iitrpr.ac.in e 8 Prof. Guo Zhanhu University of Tennessee Knoxville, USA zguo10@utk.edu
3.30 pm-4.00 pm 4.00 pm-4.30 pm 4.30 pm-5.00 pm	:	Invited Lectur Speaker : Invited Lectur Speaker : Invited Lectur	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar dmandal@iitrpr.ac.in e 8 Prof. Guo Zhanhu University of Tennessee Knoxville, USA zguo10@utk.edu e 9
3.30 pm-4.00 pm 4.00 pm-4.30 pm 4.30 pm-5.00 pm	: :	Invited Lectur Speaker : Invited Lectur Speaker : Invited Lectur Speaker :	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar dmandal@iitrpr.ac.in e 8 Prof. Guo Zhanhu University of Tennessee Knoxville, USA zguo10@utk.edu e 9 Prof. B. M. Bhanage
3.30 pm-4.00 pm 4.00 pm-4.30 pm 4.30 pm-5.00 pm	:	Invited Lectur Speaker : Invited Lectur Speaker : Invited Lectur Speaker :	rnp_1949@yahoo.co.in e 7 Prof. Debprasad Mandal IIT Ropar dmandal@iitrpr.ac.in e 8 Prof. Guo Zhanhu University of Tennessee Knoxville, USA zguo10@utk.edu e 9 Prof. B. M. Bhanage ICT-Mumbai

Seminar-1 (Day-2)
3rd August 2021 (10.00 am-6.00 pm) (IST)
Session-IV
Research Scholars' Competition (Parallel Session)
(9.30 pm-2.00 pm) (IST)
(Judges panel)
Session-V
Invited Lectures
(2.00 pm-5.30 pm) (IST)

Chairperson: Prof. R. D. Kaushik rduttkaushik@gmail.com

2.00 pm-2.30 pm	:	Invited Lecture 10	
		Speaker :	Prof. Edmana Prasad
			IIT-Madras
			pre@iitm.ac.in
2.30 pm-3.00 pm	:	Invited Lectur	e 11
		Speaker :	Prof. Rintu Banerjee
			III Kharagpur
0.00	_	L	rintuin@gmail.com
3.00 pm-3.30 pm	:	Invited Lectur	e 12 Des f. M. K. Dathard
		Speaker :	Prot. V. K. Ratnod
			ICI, Mumbal
			vk.ratnod@ictmumbai.edu.in
		Chairp	person: Prof. Anand Aswar
			aswaranand@gmail.com
3 30 pm-4 00 pm		Invited Lectur	e 13
	•	Speaker ·	Prof. Venkata Krishnan
		opeaner .	IIT Mandi, Himachal Pradesh
			vkn@iitmandi.ac.in
4.00 pm-4.30 pm	:	Invited Lectur	e 14
		Speaker ·	
		opound .	Dr. Asit K. Das
		Opeanor .	Dr. Asit K. Das Reliance Industries Ltd., Jamnagar
		opoundr .	Dr. Asit K. Das Reliance Industries Ltd., Jamnagar asit.das@ril.com
4.30 pm-5.00 pm	:	Invited Lectur	Dr. Asit K. Das Reliance Industries Ltd., Jamnagar asit.das@ril.com e 15
4.30 pm-5.00 pm	:	Invited Lectur Speaker :	Dr. Asit K. Das Reliance Industries Ltd., Jamnagar asit.das@ril.com e 15 Dr. Ashanendu Mandal
4.30 pm-5.00 pm	:	Invited Lectur Speaker :	Dr. Asit K. Das Reliance Industries Ltd., Jamnagar asit.das@ril.com e 15 Dr. Ashanendu Mandal Former Chief General Manager, ONGC
4.30 pm-5.00 pm	:	Invited Lectur Speaker :	Dr. Asit K. Das Reliance Industries Ltd., Jamnagar asit.das@ril.com e 15 Dr. Ashanendu Mandal Former Chief General Manager, ONGC ashanendumandal@gmail.com
4.30 pm-5.00 pm 5.00 pm-5.30 pm	:	Invited Lectur Speaker :	Dr. Asit K. Das Reliance Industries Ltd., Jamnagar asit.das@ril.com e 15 Dr. Ashanendu Mandal Former Chief General Manager, ONGC ashanendumandal@gmail.com e 16
4.30 pm-5.00 pm 5.00 pm-5.30 pm	:	Invited Lectur Speaker : Invited Lectur Speaker :	Dr. Asit K. Das Reliance Industries Ltd., Jamnagar asit.das@ril.com e 15 Dr. Ashanendu Mandal Former Chief General Manager, ONGC ashanendumandal@gmail.com e 16 Prof. Debabrata Mazumder

debabrata@civil.iiests.ac.in

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Seminar-2 (Day-1) Young Scientists Conclave 7th August 2021 (9.40 am-5.30 pm) (IST) 9.40 am-9.50 am : Address by Convener 9.50 am-10.00 am : Address by President, ICS

Session-I (Invited Lectures) Section: Inorganic Chemistry (9.30 am-12.30 pm) (IST)

Chairperson: Prof. Ashutosh Ghosh ghosh_59@yahoo.com

9.30 am-10.00 am	:	Inaugural Lec Speaker :	ture (Lecture-17) Prof. Kaushik Ghosh IIT Roorkee	
10 00 cm 10 20 cm		Invited Loctur		
10.00 am- 10.30 am	•			
		Speaker :	Dr. Ramanada Maity University of Calcutta, Kolkata rmchem@caluniv.ac.in	
10.30 am-11.00 am	:	Invited Lectur	Invited Lecture 19	
		Speaker :	Dr. Partha Mahata	
			Jadavpur University	
			parthachem@gmail.com	
			partilachem@gmail.com	
		Chairp	erson: Prof. Birinchi K. Das	
		F	birinchi.das@gmail.com	
11.00 am-11.30 pm	:	Invited Lectur	e 20	
•		Speaker :	Dr. Anui Sharma	
		op contor i	Central University of Rajasthan	
			aks jitk@gmail.com	
11 20 nm 12 00 nm		Invited Lectur	~ 21	
11.30 pm-12.00 pm	•		CZI Dr. Versketeck V	
		Speaker :	Dr. venkatesn v.	
			venkatesh.v@cy.iitr.ac.in	
12.00 pm-12.30 pm	:	Invited Lectur	e 22	
		Speaker :	Dr. Shabhana Khan	
			IISER, Pune	
			shabana@iiserpune.ac.in	

		Session-II Research Scholars' Competition (12.30 pm-2.30 pm) (IST) Session-III (Invited Lectures) Section: Organic Chemistry (2.30 pm-5.30 pm) (IST)			
		Chairperson: Prof. Asok Kumar Mallik mallikak52@yahoo.co.in			
2.30 pm-3.00 pm	:	Inaugural Lecture (Lecture 23) Speaker : Prof. D. Ramachary University of Hyderabad ramchary.db@gmail.com			
3.00 pm-3.30 pm	:	Invited Lecture 24 Speaker : Dr. Madhusudan Maji IIT Kharagpur msm@chem.iitkgp.ac.in			
3.30 pm-4.00 pm	:	Invited Lecture 25 Speaker : Dr. Anasuya Roychowdhury IIT Bhubaneswar aroychowdhury@iitbbs.ac.in			
		Chairperson: Prof. Pranab Ghosh pizy12@yahoo.com			
4.00 pm-4.30 pm	:	Invited Lecture 26			
		Speaker : Dr. Soumyajit Das IIT Ropar chmsdas@iitrpr.ac.in			
4.30 pm-5.00 pm	:	Invited Lecture 27 Speaker : Prof. Nitin T. Patil IISER-Bhopal npatil@iiserb.ac.in			
5.00 pm-5.30 pm	:	Invited Lecture 28			
		Speaker : Dr. Biswajit Maji IGN Tribal University, Amarkantak biswajit.maji@igntu.ac.in			

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Seminar-2 (Day-2)								
8th August 2021 (9.40 pm-6.00 pm) (IST)								
	9.40 am-9.50 am: Address by Convener							
	9.50 am-10.00 am: Address by President ICS							
	Session-IV (Invited Lectures)							
	Sec	tion: Physical Chemistry						
	(*	$10.00 \text{ am}_{-1} 00 \text{ nm}$ (IST)						
	(
	Chair	person: Prof. Anindya Datta						
		anindya@chem.iitp.ac.in						
10.00 am-10.30 am	: Inaugural Le	cture (Lecture 29)						
	Speaker :	Prof. P. A. Hassan						
		BARC, Trombay, Mumbai						
		hassan@barc.gov.in						
10.30 am-11.00 am	: Invited Lectu	ire 30						
	Speaker :	Dr. Sanghamitra Chatterjee						
		ICI, Mumbai						
11.00 am 11.20 am	· Invited Lectu							
11.00 alli=11.30 alli	Speaker · Dr Subrata Chattonadhyay							
	Opeaner .	IIT Patna						
sch@iitp.ac.in								
Chairperson: Prof. Homendra Naorem								
		naorem.homendra@gmail.com						
11.30 am-12.00 pm	: Invited Lectu	ıre 32						
•	Speaker :	Dr. Bimlesh Lochab						
		Shib Nadar University, Gautam Buddha Nagar						
		bimlesh.lochab@snu.edu.in						
12.00 pm-12.30 pm	: Invited Lectu	ire 33						
	Speaker :	Dr. Manas Bnunia Talwa Instituta of Tashnalamu Janan						
		nokyo insulule of rechnology, Japan manas huunia@gmail.com						
12.30 pm-1.00 pm	: Invited Lectu	ire 34						
.2.00 pm 1.00 pm	Speaker :	Prof. Ramesh C. Deka						
	,	Tezpur University, Assam						
		ramesh@tezu.ernet.in						
1.00 pm-1.30 pm	: Lunch Break							

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Session-V (Invited Lectures) Section: Applied Chemistry (1.30 pm-4.00 pm) (IST)

Chairperson: Prof. Sudip K. Das drsudipkdas@gmail.com

1.30 pm-2.00 pm	Inaugural Lecture (Lec Speaker : Prof. Sin IIT Khar	ture 35) rsendu De agpur
2.00 pm-2.30 pm	sde@ch Invited Lecture 36	ie.iitkgp.ac.in
F F	Speaker : Prof. Sa IISER K sayanb(iyan Bhattacharyya olkata ପ୍ରiiserkol.ac.in
2.30 pm-3.00 pm	Invited Lecture 37	
p p	Speaker : Dr. Nay Governr drs.nrs@	an Ranjan Singha nent Engineering College, Kolkata ⊉gmail.com
	Chairperson	: Dr. Anjan Ray director@iip.res.in
3.00 pm-3.30 pm	Invited Lecture 38	
	Speaker : Dr. Ana ICT Mur ar kandi	nt Kapdi nbai @ictmumbai.edu.in
3 30 pm-/ 00 pm	Invited Lecture 30	electrication and a constraints
o.oo piii 4 .oo piii	Speaker : Mr. Dipa N R Gte dipak.pa Valedic	ak K. Pahari ch Services Pvt. Ltd., Kokata ahari@nrgtechglobal.com tory Session
	4.00 pm	-6.00 pm
	Chairperson: F	Prof. G. D. Yadav
	Presentation by Cov	vid Frontline Warrior:

- Speaker : Dr. Randeep Guleria, Director, AllMS-Delhi
- Speaker : Dr. Fuad Halim, Kolkata

Declaration of Competition Results Feedback Analysis & Comments Declaration of Closing by the President

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International Seminar on Recent Advances in Chemistry and Material Sciences (2021), Young Scientist Conclave (2021) & Student Science Meet (2021)

The 160th Birth Anniversary Celebration of Acharya Prafulla Chandra Ray

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LIFETIME ACHIEVEMENT AWARD, 2020



INDIAN CHEMICAL SOCIETY LIFETIME ACHIEVEMENT AWARD, 2020 CONFERRED ON Dr. Jhillu Singh Yadav, FNA



Members of the Council and the Fellows of the Indian Chemical Society feel highly honoured to felicitate Dr. Jhillu Singh Yadav in recognition of his lifetime achievement in teaching and research in the field of Chemistry in general and Organic Chemistry in particular.

Dr. Yadav obtained Bachelor's and Master's degrees in Chemistry from Banaras Hindu University and Ph.D. degree from M. S. University, Baroda. Dr. Jhillu Singh Yadav, CSIR Bhatnagar Fellow & former Director, Indian Institute of Chemical Technology (IICT), Hyderabad carried out extensive basic and applied research investigations in organic chemistry for the synthesis of over 190 complex natural products of biological relevance. Dr. Yadav specializes in the state-of-the art Asymmetric Synthesis to create new Chiral Centers. He extensively utilized them very effectively in the synthesis of drugs and agrochemicals having self-defensive properties against rice-blast disease, hypersensitive metabolites, anticancer, antibiotics and antifungal agents in a highly innovative manner. He excelled in creating and generating diverse chemical entities relevant to both agro and drug industry.

The insightful instincts of Dr. Yadav made him to foresee the versatility of insect sex pheromones in Indian agro-system. He pioneered the alternative eco-friendly and environmentally safe pest control technologies in India through the application of insect pheromones as major tools in Integrated Pest Management (IPM) for better and cleaner agro-products. His technology development efforts are highly commendable.

Some of the drugs developed by Dr. Yadav have been well received by several Indian Industries like Diltiazem, Ketotifen, Mefloquin, Ondasetron (Cipla), Pyrazinamide (SPIC Pharma), Tamoxifin (Cipla) Misoprostol and Carboprost (AVRA Laboratories) etc.

Dynamic leadership of Dr. Yadav created and formulated many interdisciplinary programs at the Institute with the distinct aim to serve the nation. These have since established themselves as centers of excellence at the Institute.

Dr. Yadav is an architect of distinction in building potential research groups with state-of- the-art facilities. He is an outstanding Organic Chemist of India. The Web of science (Science Citation Index) has referred him as the best and organic chemist par excellence in the country.

Dr. Yadav has the unique distinction of excelling in both basic and industrial research and received recognition accordingly. He is a fellow of The World Academy of Sciences (TWAS) for the advancement of science in developing countries and has received numerous national and international awards which include the prestigious, Shanti Swarup Bhatnagar Prize, Vigyan Gaurav Samman Award, Jawaharlal Nehru Science Award, Ranbaxy Award, Vasvik Award, Goyal Award, CSIR Technology Award, KIA Award (Iran-UNESCO). He is also the fellow of all the Indian Science Academies.

A dedicated academician, Dr. Yadav has contributed significantly to the development of Chemical Education and Research in the country. Dr. Yadav has built up a vibrant school of chemists and inspired a large number of students and colleagues who are carrying the torch of his mission. Two hundred and forty students have received their Ph.D. degrees under his able guidance in Organic Chemistry. To his credit, he has more than 1200 scientific publications with 30000 citations and 140 patents.

The Indian Chemical Society sincerely wishes Dr. Jhillu Singh Yadav a long peaceful life with sound health and continuous academic activities for the advancement and propagation of scientific knowledge.

Professor G. D. Yadav President Indian Chemical Society Professor Chittaranjan Sinha Honorary Secretary Indian Chemical Society

Keynote Address

Excitement in the synthesis of natural products

J. S. Yadav (former Director and Bhatnagar Fellow, CSIR-IICT) Provost, Director and Trustee, Indrashil University, Ahmedabad-382 740, Gujarat, India Email : jsyadav@iist.edu.in yadavfna@gmail.com



At a time when scientific community was trying more than ever to harness the potential and promise of organic chemistry towards the preparation of organic compounds, one can't discuss about the asymmetric synthesis without mentioning his visionary and powerful application of chiral approach. As part of his interest in the asymmetric total synthesis of natural products and their analogues, extensive research has been carried out by his group to develop a desymmetrization approach giving rise to five contiguous chiral centers with excellent diastereoselective manner, directed-Prins cyclization protocol for the synthesis of 2,4,6-syn-trisubstituted tetrahydropyran derivatives under environmentally benign conditions and further transformations for the formation of anti-1,3-diol, Sakurai-type allylation towards the synthesis of substituted tetrahydrofurans and tetrahydropyrans, highly enantioselective synthesis of propargyl alcohol derivatives from epoxy alcohol and carbohydrates paved the way to major developments in the utilization of these protocols for the total syntheses of a variety of complex biologically active natural products. In order to address the arbitrary use of harmful pesticides, his group pioneered Pheromone Application Technology (PAT) by utilizing insect pheromones, the chemicals released by insects for communication and behavioural response, which will be discussed during the presentation.

Brief Bio-Sketch

Dr. Jhillu Singh Yadav, Provost, Director and Trustee, Indrashil University (former CSIR Bhatnagar Fellow & Director, Indian Institute of Chemical Technology (CSIR-IICT)), Hyderabad carried out extensive basic and applied research investigations in organic chemistry for the synthesis of over 190 complex natural products of biological relevance. Dr. Yadav specializes in the state-of-the art Asymmetric Synthesis to create new Chiral centers. He extensively utilized them very effectively in the synthesis of activities of drugs and agrochemicals having self-defensive properties against rice-blast disease, hypersensitive metabolites, anticancer, antibiotics and antifungal agents in a highly innovative manner. He excelled in creating and generating diverse chemical entities relevant to both

agro and drug industry. Dr. Yadav's insightful instincts made him foresee the versatility of insect sex pheromones in Indian agro-system. He pioneered the alternative eco-friendly and environmentally safe pest control technologies in India through the application of insect pheromones as major tools in Integrated Pest Management (IPM) for better and cleaner agro-products. The pheromone application technologies include the control of pests on cotton, rice, groundnut and other vegetable crops. His technology development efforts are highly commendable. Dr. Yadav successfully developed costeffective technologies for drugs which have been well received by several Indian Industries like Diltiazem, Ketotifen, Mefloquin (Cadila Pharma) Ondasetron (Cipla), Pyrazinamide (SPIC Pharma), Tamoxifin (Cipla) Misoprostol and Carboprost (AVRA Laboratories) etc.

His dynamic leadership could create and formulate many interdisciplinary programs at the Institute with the distinct aim to serve the nation. These have since established themselves as centers of excellence at the Institute. They include exploration of natural products/herbal products for health care, novel inputs for integrated pest management, advanced applications of chemical biology for therapeutics, state-of-the-art research and development facilities in the area of lipids and development of green processes technologies based on advanced catalysis.

Dr. Yadav is an architect of distinction in building potential research groups with state-of-the-art facilities. He is an outstanding Organic Chemist of India. The Web of science (Science Citation Index) has referred him as the best and organic chemist par excellence in the country. His vibrant research group is a center for developing quality scientific human resources. More than 250 students have received their Ph.D. degrees under his able guidance in organic chemistry. To his credit, he has more than 1250 scientific publications with 25000 citations. Dr. Yadav has the unique distinction of excelling in both basic and industrial research and received recognition accordingly. He is a fellow of The World Academy of Sciences (TWAS) for the advancement of science in developing countries and has received numerous national and international awards which include the prestigious, Shanti Swarup Bhatnagar Prize, Vigyan Gaurav Samman Award, Jawaharlal Nehru Science Award, Ranbaxy Award, Vasvik Award, Goyal Award, CSIR Technology Award, KIA Award (Iran-UNESCO). He is also the fellow of all Indian Science Academies. Dr. Yadav is an eminent organic chemist with a high level of commitment to his profession. He is an avid researcher, an inspiring leader and truly an institution builder.

Endowment Lecture

Endowment Lecture Acharya P. C. Ray Memorial Lecture (2019)

Organometallic complexes of the platinum metals: Synthesis and utilization

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Transition metal promoted chemical transformation of organic molecules has been of considerable current interest. Such transformation often proceeds via a metal-carbon bond formation step, generating an organometallic complex as the reactive intermediate, which then undergoes further reactions to yield the final product(s). Synthesis of organometallic complexes and exploration of their properties are thus of significant importance. Formation of M-C bonded species may be achieved by simple σ -coordination of C-donor ligands (such as CO and NHCs), or via binding olefins or arenes to metal centers in a π -fashion. The other popular way for synthesis of M-C σ -bonded complexes is via C-H, C-C, or C-X (X = Cl, Br, etc.) bond activations of organic ligands.

Through our efforts toward formation of M-C σ -bonded species via C-H, C-C, or C-halogen atom bond activations, we have learnt that success of such an attempted metal-carbon bond formation reaction depends largely on the choice of organic ligands as well as of the metalcontaining starting materials. We have also experienced that, in many cases, the obtained results differ significantly from the expectations. In this talk some of our observations on the formation of organometallic complexes of selected platinum metals will be presented. Utilization of the organometallic complexes as catalysts in bringing about organic transformations will also be described.

Utilization of organometallic species as chemotherapeutics for combating certain diseases, cancer in particular, has been gaining prominence. Platinum metal-based organometallic complexes are known to find wide application as anti-cancer agents. The ongoing efforts in this area are focused toward development of new platinum metal-based anticancer complexes with minimal side effects and, high selectivity and cytotoxicity toward cancer cells. Some recent results from our group in this area will be shared.

Brief Bio-Sketch

Prof. Samaresh Bhattacharya is a Professor of Department of Chemistry, Inorganic Chemistry Section, Jadavpur University, Kolkata, India. He did his B.Sc. and M.Sc. from Jadavpur University on 1978 and 1980 respectively. He did his Ph.D. from IACS under the supervision of Prof. A. Chakraborty on 1986. Then he moved to University of Colorado at Boulder, USA for his postdoctoral research work from 1988 to 1991. He started his independent research work from Department of Chemistry, Jadavpur University on the year of 1992. His area of research is Coordination chemistry of the platinum group of metals, Organometallic chemistry, Catalysis. He has published 152 papers. He has guided 30 students to get their Ph.D. degree. He has achieved many prestigious awards and recognitions. He has received S. S. Bhatnagar Prize in 2005, bronze medal from the Chemical Research Society of India in 2006. He has Elected Fellow of the Indian Academy of Sciences in 2006. He has Elected Fellow of the Indian Academy of Sciences in 2006. He has Secience & Technology in 2008. He is Awarded with the Ramanna Fellowship of DST in 2009, "Acharya P. C. Ray Memorial Award for the year 2019" by the Indian Chemical Society. He is the Life member of the Indian Chemical Society, Indian Association for the Cultivation of Science and the Chemical Research Society of India.

Invited Lectures

[1 - 40]

Invited Lecture-1

Total synthesis of architecturally complex natural products as a platform for the discovery of novel methodologies under aerobic oxidation

Alakesh Bisai



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Nature produces a variety of complex natural products and majority of these are isolated in entioenriched form (e.g. alkaloids **1-3**)¹. Since these are isolated from Nature in limited quantity (mostly in mg scale), total synthesis endeavors can play a crucial role in bioactivity evaluation by providing access to significant quantity. It also provides platform for the innovation of new strategies for chemical synthesis. Further, catalytic asymmetric construction of organic molecules sharing all-carbon quaternary stereocenter (see, **3-5**) is one of the challenging aspects of synthetic organic chemistry².



Figure. Architecturally intriguing indole alkaloids of biological relevance.

Towards this direction, naturally occurring alkaloids (Figure) with impressive diversity of biological activities drew our interest for efficient total syntheses^{1a}. Interestingly, a variety of alkaloids of this family show antibacterial and cytotoxic activities^{1b}. In order to devise strategy of above targets³, we explored novel methodologies that addresses core structure of these

interesting alkaloids under mild condition⁴. Our endeavors towards the total syntheses⁵ of architecturally intriguing natural products via oxidative transformations will be discussed⁶.

References

- Reviews: (a) J. Mulzer, T. Gaich and P. Siengalewicz, *Angew. Chem., Int. Ed.*, 2008, **47**, 8170; (b) D. Greiner, T. Bonaldi, R. Eskeland, E. Roemer and A. Imhof, *Nat. Chem. Biol.*, 2005, **1**, 143; (c) S. De, S. Ghosh, S. Bhunia, J. A. Sheikh and A. Bisai, *Org. Lett.*, 2012, **14**, 4466.
- (a) S. Ghosh, L. K. Kinthada, S. Bhunia and A. Bisai, *Chem. Commun.*, 2012, 48, 10132; (b) S. Ghosh, S. De, B. N. Kakde, S. Bhunia, A. Adhikary and A. Bisai, *Org. Lett.*, 2012, 14, 5864; (c) S. Bhunia, S. Ghosh, D. Dey and A. Bisai, *Org. Lett.*, 2013, 14, 2426.
- (a) S. Ghosh, S. Bhunia, B. N. Kakde, S. De and A. Bisai, *Chem. Commun.*, 2014, **50**, 2434; (b) S. Ghosh, S. Chaudhuri and A. Bisai, *Org. Lett.*, 2015, **17**, 1373; (c) B. N. Kakde, N. Kumar, P. K. Mondal and A. Bisai, *Org. Lett.*, 2016, **18**, 1752; (d) S. Ghosh, S. Chaudhuri and A. Bisai, *Chem.-Eur. J.*, 2015, **21**, 17479.
- (a) S. De, M. K. Das, S. Bhunia and A. Bisai, *Org. Lett.*, 2015, **17**, 5922; (b) S. Ghosh, S. Chaudhuri and A. Bisai, *Chem.-Eur. J.*, 2015, **21**, 17479; (c) N. Babu, A. Roy, M. Singh and A. Bisai, *Org. Lett.*, 2018, **20**, 6327; (d) M. K. Das, N. Kumar and A. Bisai, *Org. Lett.*, 2018, **20**, 4421.
- (a) N. Kumar, M. K. Das, S. Ghosh and A. Bisai, *Chem. Commun.*, 2017, **53**, 2170; (b) S. Bhunia, S. Chaudhuri and A. Bisai, *Chem.-Eur. J.*, 2017, **23**, 11234; (c) N. Babu, L. K. Kinthada, P. P. Das and A. Bisai, *Chem. Commun.*, 2018, **54**, 7963.
- (a) A. Roy, M. K. Das, S. Chaudhuri and A. Bisai, *Chem. Commun.*, 2018, **54**, 940; (b) S. Chaudhuri, S. Bhunia, A. Roy, M. K. Das and A. Bisai, *Org. Lett.*, 2018, **20**, 288; (c) N. Kumar, A. Maity, V. R. Gavit and A. Bisai, *Chem. Commun.*, 2018, **54**, 9083.

Brief Bio-Sketch

After receiving M.Sc. degree in Organic Chemistry from Banaras Hindu University, Alakesh obtained his Ph.D. in synthetic Organic Chemistry under the supervision of Professor Vinod K. Singh from the Department of Chemistry, Indian Institute of Technology Kanpur in Sept. 2006. Immediately afterward, he moved to the College of Chemistry, University of California at Berkeley, where he held postdoctoral position in the research group of Professor Richmond Sarpong. During his stay at Berkeley, he completed concise total synthesis of *'lycopodium alkaloids'* lyconadin A which received considerable attention from the synthetic community. During his Postdoctoral research, he received the GRC (*Gordon Research Conference*) award to Post-docs by Chair, 17th GRC on Stereochemistry (2008), RI. In Dec. 2009, he left Berkeley and joined IISER Bhopal as an Assistant Professor, where he had been serving as a Professor in the Department of Chemistry till May, 2020. In May, 2020, he moved to the Department of Chemical Sciences, IISER Kolkata to set a research lab. on Natural Product synthesis of architecturally interesting biologically active natural products that provide an ideal platform for the invention of new strategies and highly selective organic transformations. A number of naturally occurring architecturally interesting biological relevant secondary metabolites sharing all-carbon quaternary

stereocenters have been synthesized by his research group. Recently, his total synthesis of pyrroloindoline alkaloids had been highlighted in '*Organic Chemistry Portal* as '*The Bisai Synthesis of (–)-Physovenine*'. He had been invited to deliver several invited lectures in India and abroad, to name a few, FloHet-2020 (USA), Georgetown Univ. (2020), INDIGO-2015 (Germany), BASF-2015 (Ludwigshafen, Germany), Gregynog-2013 (Wales, UK), Univ. of Bath, UK (2013), Cardiff Univ., UK (2013) and many important conferences held in India. His research has been appreciated in the form of various awards and honours, to name a few notable ones:SERB-STAR Award (2021-2024), CRSI Bronze Medal (2021), Fellow, Indian Chemical Society (FICS-2020), CRSI Young Scientist Award (2018), Lead Lecture (Junior) at 'Pfizer Symposium', IISc (2016), DST Young Scientist Research Grant (2013), BRNS Young Scientist Award & Grant (2011), GRC Award to Post-doc. by Chair (2008), He had served IISER Bhopal in different administrative capacities as below (major activities):Chief Vigilance Officer (CVO), Dean of the Faculty Affairs (DoFA), Chairperson, Health Center User Committee (HCUC), Member, Departmental Faculty Advisory Committee (DFAC), Conveners, DUGC and DPGC, Chemistry, Coordinator, Outreach Activities.

Invited Lecture-2

The magic of two aqueous layers in contact and beyond



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Aqueous solutions have an immense potential to show mutual incompatibility and separate into immiscible layers resulting in aqueous biphasic systems (ABSs). They were first perceived way back in 1896 when its mere possibility was observed by Martinus Willem Beijerinck. However, the immense capability of these systems towards addressing several analytical problems was revealed much later. ABSs present all the qualities of solvent extraction but are free from toxic and hazardous organic solvents. Water soluble polymers, salts, amino acids, carbohydrates and even alcohols have shown the capacity to form mutually immiscible phases. Applications of ABSs first began with separation of different biomolecules which increased in the later years in leaps and bounds in separating cells, dyes, nanoparticles and several other analytes. Extraction and separation of metal ions using ABSs were then taken up which showed competence in separating mutually related metal species with judicious modulation of physical parameters. Optimum conditions for separation is found to depend on factors like pH, temperature, concentration of the phase forming components, polymer chain length and so on. Recent studies have also directed towards some new aspects of the fields of application of ABSs. These are towards the identification of molecular interactions which can occur between different drugs, or biomolecules or any other kind of molecules that may result in unexpected outcomes. The discussion on this topic will encompass several such issues and their recent advances.

Brief Bio-Sketch

Dr. Kamalika Sen is working as an Assistant Professor in the Department of Chemistry, University of Calcutta since 2010. Her main research interest is in the field of Analytical Chemistry. Her research topics entail different aspects of the subject like development of green methodology for speciation of elements in the ultra trace scale, exploring different aqueous two phase extraction systems, separation of protein fractions from peanut and their interactions with metal ions, developing green methodology

for synthesis of nanoparticles and effect γ radiation. Currently her interest is focused on development of different porous materials. She has received various grants from UGC, DST and UGC-DAE for her research. Till now 8 students have obtained their PhDs under her supervision. She is currently supervising 4 Ph.D. students and 2 Post doctoral fellows. She has published around 106 articles in International journals.

Invited Lecture-3

Discovering new crystalline forms via cocrystallization

Deepak Chopra



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Cocrystal formation is an important technique of extreme relevance in the design of new pharmaceuticals¹. Organic multicomponent crystals, such as co-crystals and salts, are of interest in the pharmaceutical industry², due to the possibility of improved physicochemical properties in comparison to their constituent species³.

The current talk shall address the applications of mechanochemical synthesis, via cocrystallization, in the anti-diabetic drug chlorpropamide $(cpa)^4$. An organic salt was formed with 4-(dimethylamino)pyridine (*cpa:DMAP*) and a cocrystal was obtained with 4,4' -dipyridyl (*cpa:BP*). After extensive screening for polymorphism/stoichiomorphism, two polymorphs of the *cpa:DMAP* salt (Forms I and II) and one form of the cocrystal *cpa:BP* were discovered. *cpa:DMAP-I* crystallized with eight molecules in the asymmetric unit (Z' = 4, Z'' = 8), whereas *cpa:DMAP-I* crystallized with two molecules in the asymmetric unit (Z' = 1, Z'' = 2). It was also observed that the stable polymorph of the salt *cpa:DMAP-I* has a drastically enhanced aqueous solubility and dissolution rate relative to the pure *cpa*, thus giving it an advantage for improved drug delivery.

References

- 1. S. R. Byrn, G. Zografi and X. Chen, *Solid State Properties of Pharmaceutical Materials*, John Wiley & Sons, Inc., Hoboken, 2017.
- 2. Y.-M. Yu, L.-Y. Wang, F.-Z. Bu, L.-L. Wang, Y.-T. Li, C. Wang and Z.-Y. Wu, *CrystEngComm.*, 2020, **22**, 7992.
- 3. C. Aakeröy, Acta Crystallogr., Sect. B: Struct. Sci., Cryst. Eng. Mater., 2015, 71, 387.
- 4. B. Haripriya, A. Hasija, A. J. Cruz-Cabeza, I. Shruti and D. Chopra, *Cryst Growth & Des.*, 2021, In Press (https://doi.org/10.1021/acs.cgd.1c00236).

Brief Bio-Sketch

Dr. Deepak Chopra is currently Associate Professor in the Department of Chemistry at Indian Institute of Science Education and Research (IISER) Bhopal, Madhya Pradesh since March 2009. He received his degree in B.Sc. (H) Chemistry (Gold Medallist) from Jadavpur University in 2001. Following which he pursued the Integrated Ph.D. program (which includes a 3 year M.S. program) from Indian Institute of Science, Bangalore in Chemical Crystallography. He continued as a postdoctoral fellow in IISc till 2007. He further continued his postdoctoral work at the University of Toledo, Ohio, USA in the field of electron density analysis in molecular crystals. His active research interests, includes investigation of polymorphism in drugs and pharmaceuticals, computational analysis of non-covalent interactions, *in situ* crystallization, experimental/theoretical electron density analysis and mechanical/electrical properties in molecular crystals. He is currently on the Editorial Board of *Journal of Molecular Structure*, Elsevier, a Co-Editor of the journal *Acta Crystallographica E* (IUCr, Chester), a *Fellow* of the *Indian Chemical Society* (FICS) and a *Fellow* of the *Royal Society of Chemistry* (FRSC).
Strategic design and development of nanostructured heterogeneous catalysts for clean energy and environmental applications



Venkata Krishnan

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Energy crisis and environmental deterioration has emerged as a major problem around the world in recent times, mainly due to combustion of fossil fuels and their depletion. The utilization of solar energy for the production of chemical fuels is an attractive and major strategy to address the global energy crisis and other environmental issues. The design and development of highly efficient, eco-benign and cost-effective photocatalysts, which can utilize the naturally abundant solar light, is highly desired for energy generation through water splitting and environmental remediation through the degradation of pollutants. Our research group has recently developed several two dimensional carbon (reduced graphene oxide and graphitic carbon nitride) supported nanostructured photocatalysts based on semiconductors, plasmonic materials, perovskite structures and upconversion nanoparticles, which can utilize the full solar spectrum from ultraviolet to infrared regions for energy generation and environmental remediation applications. In addition, our group has also developed efficient Green catalysts for organic transformation reactions to synthesize medicinally relevant indole alkaloids in water. Furthermore, our group has also worked on the development of bioinspired scaffolds for heterogeneous catalysis and also on the development of carbon based catalysts for biomass conversion. The highlights of the ongoing research works of our group will be presented.

References

- 1. A. Kumar and V. Krishnan, Adv. Func. Mater., 2021, doi: 10.1002/adfm.202009807.
- 2. A. Kumar, A. Kumar and V. Krishnan, ACS Catal., 2020, 10, 10253.
- 3. A. Kumar, K. R. Shankar, A. Kumar, G. Harith and V. Krishnan, *J. Environ. Chem. Eng.*, 2021, **9**, 105147-1-13.
- 4. A. Kumar, P. Choudhary, K. Kumar, A. Kumar and V. Krishnan, Mater. Chem. Front., 2021, 5, 1448.
- 5. A. Kumar, V. N. Rao, A. Kumar, A. Mushtaq, L. Sharma, A. Halder, S. K. Pal, M. V. Shankar and V. Krishnan, *ACS Appl. Ener. Mater.*, 2020, **3**, 12134.

- P. Choudhary, A. Bahuguna, A. Kumar, S. S. Dhankar, C. M. Nagaraja and V. Krishnan, *Green Chem.*, 2020, 22, 5084.
- 7. T. Chhabra, A. Bahuguna, S. S. Dhankhar, C. M. Nagaraja and V. Krishnan, *Green Chem.*, 2019, **21**, 6012.
- S. Kumar, A. Kumar, V. N. Rao, A. Kumar, M. V. Shankar and V. Krishnan, ACSAppl. Energy Mater., 2019, 2, 5622.

Dr. Venkata Krishnan completed his Ph.D. in Physical Chemistry in 2006 at the University of Stuttgart, Germany. Subsequently, he worked as a postdoctoral researcher at the University of Pennsylvania, USA from 2006 to 2010 and then as a research associate at the National Institute for Materials Science (NIMS), Japan from 2010 to 2012. He joined as a faculty at the Indian Institute of Technology (IIT) Mandi in April 2012. His research group is mainly working in the field of heterogeneous catalysis for energy and environmental applications. He has successfully guided 4 Ph.D. and 15 M.Sc. students and is currently guiding 8 Ph.D. and 5 M.Sc. students, in addition to several short term research interns. He has published more than 130 research articles in well reputed international journals and is also a reviewer for several scientific journals. He has been bestowed with several awards, including DST INSPIRE faculty award, IIT Mandi foundation day award for excellence in teaching, MANA research fellowship, DoE postdoctoral fellowship, DFG doctoral fellowship, DAAD visiting scholar fellowship, etc. In addition to teaching and research, he has also served IIT Mandi in various administrative positions, such as first warden of the hostel in main campus, founding head of Advanced Materials Research Center (AMRC), Associate Dean Research, etc. Currently, he is serving as the Dean of Sponsored Research, Industrial Consultancy and International Relations at IIT Mandi.

Stabilization of Polyoxometalates towards electrocatalysis extremely harsh conditions



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Polyoxometalates (POMs) are extensively used as efficient catalyst in water oxidation, electrocatalysis, energy storage, biomolecule sensing and organic transformations due to their structural diversity, robustness and multi-electron redox properties. However, the stability and redox activity of POMs is highly pH dependent. We are particularly interested on sandwich POMs, due to their well-defined and easy accessible catalytic sites and are better catalysts than simple keggin POMs. A detail stability and reactivity of sandwich POMs were studied prior to electrocatalytic applications. However, these sandwich POMs are unstable either in alkaline (pH > 8) or acidic (pH < 5) media.



Figure. Ionic polymer supported sandwich POMs toward electrocatalytic applications.

Here we discuss the stabilization of different sandwich POMs with ionic polymer support under extremely harsh condition electro-catalysis like

- 1. Water oxidation in highly alkaline media (1 *M*KOH).
- 2. HCl electrolysis in highly acidic media (5 *M* HCl).

3. Cathode in Li-S battery for faster kinetics.

References

- 1. V. Singh, S. D. Adhikary, A. Tiwari, D. Mandal and T. C. Nagaiah, *Chem. Mater.*, 2017, 29, 4253.
- 2. S. D. Adhikary, A. Tiwari, T. C. Nagaiah and D. Mandal, *ACS Appl. Mater. Interfaces,* 2018, **10**, 38872.
- 3. V. Singh, A. K. Padhan, S. D. Adhikary, A. Tiwari, D. Mandal and T. C. Nagaiah, *J. Mater. Chem. (A)*, 2019, 3018.

Brief Bio-Sketch

Dr. Debaprasad Mandal did Ph.D. from the IIT Kanpur, India in 2006. He joined the IIT Ropar in 2010 as an Assistant Professor. Prior to join IIT Ropar, Dr. Mandal worked at Erlangen, Germany as an Alexander von Humboldt fellow and then he moved to Texas A & M University as senior scientist. Currently his group is focused on the development of new ionic liquids, ionic polymers, fluorous materials for catalysis, membrane towards fuel cells, Li-ion and Li-S battery. The group is extensively working on polyoxometalates for electrochemical water oxidation and greener oxidation of organic compound.

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The sizzling chemistry of silylene supported coinage metal complexes





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Development of new ligands to regulate the reactivity is of fundamental interest in transition metal catalysis. Of late, N-heterocyclic silylenes are emerging as a new class of steering ligands. Silylene transition metal complexes have been explored as catalysts for many important organic transformations and proven to be superior at several instances than classical ligands¹. Usually, the transition metals involved in these reactions are Mn, Fe, Ni, Co, Rh, Ir, Pd, Pt etc. It is apparent that although silylenes have excelled in TM chemistry, they have surprisingly not been used as ligands in homogeneous catalysis mediated by the coinage metals (Cu, Ag, Au). Given our recent interests in silylene-coinage metal chemistry², we have embarked into the silylene-Au(I)/Ag(I)/Cu(I) complexes and utilized them as catalysts in click reaction, A³ coupling reaction and polysaccharide synthesis.



References

- 1. Yu-P. Zhou and M. Driess, *Angew. Chem. Int. Ed.*, 2019, **58**, 3715.
- (a) N. Parvin, S. Pal, J. Echeverría, S. Alvarez and S. Khan, *Chem. Sci.*, 2018, 9, 4333; (b) S. Khan, S. Pal, N. Kathewad, I. Purushothaman, S. De and P. Parameswaran, *Chem. Commun.*, 2016, 52, 3880; (c) S. Khan, S. Ahirwar, S. Pal, N. Parvin and N. Kathewad, *Organometallics*, 2015, 34, 5401.

Brief Bio-Sketch

Shabana Khan obtained her Ph.D. degree from the Indian Institute of Technology, Delhi in 2008 under the supervision of Prof. Jai Deo Singh in the area of organoselenium chemistry. Subsequently, she received the fellowship of Deutscher Akademischer Austausch Dienst (DAAD) and joined the research group of Prof. Herbert W. Roesky as a postdoctoral fellow, followed by a second post-doc with Dr. Manuel Alcarazo at the Max Planck Institute for Coal Research. She joined IISER Pune as Assistant Professor in 2013. Currently, she is working as an Associate Professor in the Department of Chemistry, Indian Institute of Science Education and Research, Pune, India. She also serves as a member of editorial advisory board of *Organometallics* (ACS). Her research interest includes the synthesis and application of compounds with low valent elements in catalysis.

Homo- and heterobimetallic N-heterocyclic carbene complexes: Employed in catalysis



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N-Heterocyclic carbenes (NHCs) have emerged as a useful class of ligands in organometallic chemistry¹. Although the majority of these ligands are based on imidazol-2ylidenes or 1,2,4-triazol-5-ylidenes (normal NHCs), their mesoionic counterparts, 1,2,3-triazol-5-ylidenes, are currently gaining immense popularity². The design and synthesis heterobimetallic NHC complexes on poly-NHC ligand platform have also received much attention owing to their applications as catalysts in cooperative or tandem catalysis³. We present here the synthesis of the cyclometalated heterobimetallic complexes with Ir(III) and Pd(II). The heterobimetallic Ir(III)/Pd(II) complex shows much higher yields in tandem C-C coupling/transfer hydrogenation reactions compared to the equimolar mixture of their mononuclear Pd(II) and Ir(III) counterparts^{4,5}.



Scheme 1. Synthesis and application of homo- and heterobimetallic complexes.

References

- 1. F. E. Hahn and M. C. Jahnke, Angew. Chem. Int. Ed., 2008, 47, 3122.
- 2. A. Zanardi, R. Corberán, J. A. Mata and E. Peris, Organometallics, 2008, 27, 3570.

- 3. J. A. Mata, F. E. Hahn and E. Peris, *Chem. Sci.*, 2014, 5, 1723.
- 4. A. Majumder, R. Naskar, P. Roy and R. Maity, Eur. J. Inorg. Chem., 2019, 1810.
- 5. A. Majumder, T. N. Saha, N. Majumder, R. Naskar, K. Pal and R. Maity, *Eur. J. Inorg. Chem.*, 2021, 1104.

Dr. Ramananda Maity was born in 1986 and did his schooling from his native place Paschim Medinipur, West Bengal. He completed B.Sc. in Chemistry (honours) from University of Calcutta in 2007 and MSc in Chemistry from IIT Madras in 2009. Dr. Ramananda Maity obtained his Ph.D. in 2013 from University of Münster under the guidance of Professor F. E. Hahn. After the first postdoctoral studies with Professor Biprajit Sarkar at Freie Universität Berlin, he joined Prof. S. Inoue at Technische Universitatät Berlin for his second postdoctoral studies. He started his first independent carrier as an Assistant Professor at Dibrugarh University in 2015. In 2016 he moved to University of Calcutta as an Assistant Professor.

Advanced chemical technologies for water and wastewater treatment



Debabrata Mazumder

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The chemical wastewater treatment processes include various processes that utilize chemicals to bring various water quality parameters within safe limits of drinking or disposal. These are necessary steps for treatment processes in lowering colloidal solids, certain organics and microorganism concentration. The processes can be categorized into chemical precipitation including coagulation and flocculation, neutralization, chemi-sorption, and disinfection. Various advanced oxidation processes help in increasing biodegradability of recalcitrant compounds thereby achieving better removal during biological process. With the advancement of technologies, these conventional processes and chemicals are being modified for driving out the disadvantages along with obtaining better removal efficiency. The use of inorganic and organic coagulants together in different proportions is one such example, which combines the advantages of both chemicals minimizing the disadvantages.

Brief Bio-Sketch

Debabrata Mazumder did his Bachelor's and Master's Degree in Civil Engineering from Jadavpur University in 1993 and 1996 respectively. He received his Ph.D. Degree in Environmental Engineering from Bengal Engineering and Science University, Shibpur (*presently I.I.E.S.T., Shibpur*) in 2004. He has a total 28 years of industrial, teaching and research experience. He published more than 120 technical papers and 5 Book Chapters in various national and international journals and conference proceedings. He is the Affiliate Member of American Society of Civil Engineers (ASCE) and the Member of International Water Association (IWA). He is also the Life Fellow of Institution of Engineers (India) (IE, India) and the Life Fellow of Institution of Public Health Engineers (India) (IPHE, India). Apart from these he is the Life Member of Indian Water Works Association (IWWA). He has supervised 4 Nos. of Ph.D. (Engg.) and 25 Nos. of M.Tech. Thesis in the field of Environmental Engineering. He acted as a Consultant in National Mission for Clean Ganga (NMCG) and National River Conservation Directorate (NRCD) under Ministry of Environment, Forests and Climate Change, GOI. He has been granted one Indian Patent titled "Shaft-type Hybrid Bioreactor". He is presently serving as the Professor of Civil Engineering Department, Indian Institute of Engineering Science and Technology, Shibpur.

Confinement of a thermodynamically stable Mono(aquated) Mn(II)-complex within a porous silica nanosphere renders a potential dual-mode MRI contrast agent



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Contrast agent enhanced magnetic resonance imaging has emerged as an indispensable imaging modality for the early-stage diagnosis of many diseases. Nevertheless, the development of stable contrast agents with a high relaxivity remained the challenge. In this endeavor, a mononuclear, mono(aquated), thermodynamically stable [log K_{Mnl} = 14.80(7) and pMn = 8.97] Mn(II)-complex (1); based on a hexadentate pyridine-picolinate unitscontaining ligand (H₂PyDPA); were synthesized and confined within a porous silica nanosphere in non-covalent fashion. The entrapped complex 1 (complex 1@SiO₂) exhibits $r_1 = 8.46 \text{ mM}^{-1} \text{ s}^{-1}$ and $r_2 = 33.15 \text{ mM}^{-1} \text{ s}^{-1}$ at pH = 7.4, 25°C, 1.41 T in HEPES buffer. The synthesized complex 1@SiO₂NP interacted significantly with albumin protein and consequently, boosted both the relaxivity values to $r_1 = 24.76 \text{ mM}^{-1} \text{ s}^{-1}$ and $r_2 = 63.96 \text{ mM}^{-1}$ s^{-1} at pH = 7.4, 37°C, 1.41 T. The kinetic inertness of the entrapped molecules was established by recognizing no appreciable change in the r_1 value upon challenging complex 1@SiO₂NP with 30 and 40 times excess of Zn(II) ions at pH 6, 25°C. The water molecule coordinated to the Mn(II) ion in complex 1@SiO₂ was also impervious to the physiologically relevant anions (bicarbonate, biphosphate, citrate) and pH of the medium. The concentration-dependent changes in image intensities in T_1 - and T_2 -weighted phantom images put forward the biocompatible complex 1@SiO₂NP as a potential dual-mode MRI contrast agent. The synthesis and contrast ability of the developed new nanosystem would be discussed in detail.

Brief Bio-Sketch

Dr. Chandan Mukherjee is a Professor of Department of Chemistry, Indian Institute of Technology Guwahati, Assam, India. He was an Associate Professor at Indian Institute of Technology Guwahati

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from 2015 to 2019. Before that he was an Assistant Professor at Indian Institute of Technology Guwahati from 2011 to 2015. He did his first postdoctoral research work in Chemistry from Max-Planck-Institut für Bioanorganische Chemie, Germany from 2007 to 2010. He did his second postdoctoral research work from The Tokyo University, Tokyo, Japan and Universität Bielefeld, Germany, Germany from 2010 to 2011. He did his doctoral work from Max-Planck-Institut für Bioanorganische Chemie, Germany from 2003 to 2007. He has got several awards and fellowshps like – Associate, Indian Academy of Science, Bangalore (2015-2018), DFG-Fellowship for postdoctoral study (2007-2010, German Research Society), DFG-Fellowship for doctoral study (2003-2006, German Research Society), National Scholarship (2001, Govt. of India), National Scholarship (1998, Govt. of India).

Ultrasound-assisted enzyme catalyzed synthesis of flavors

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The flavor esters have a fruity flavor and pleasant floral aroma and are broadly used in the food flavor and fragrance sector. As consumers' concern for health issues increases, chemical-free products are gaining more attention in the food and flavor sector than chemical catalyzed products. Biocatalysis presents a clear advantage compared to the chemical synthesis route when it comes to process operation, product purity, and a decrease in the formation of side products. Thus, biocatalysis has attracted the attention of researchers for the synthesis of various value-added flavor esters, which have wide applications in industries. However, the conventional enzymatic synthesis process requires a longer time and higher cost due to higher enzyme costs. Therefore, there is a need for a green and novel synthesis strategy to overcome these limitations. The application of process intensification tools like ultrasound can help to overcome these drawbacks by cavitation phenomenon. It is observed that the application of ultrasound improves enzyme activity and increases the reaction rate. Here, we will explore the application of ultrasound as an intensification tool for the enzyme catalyzed synthesis of flavors/perfume.

Brief Bio-Sketch

Dr. Virendra Kisan Rathod is a Professor of Institute of Chemical Technology (ICT), Matunga, Mumbai. He was an Assistant Professor at Chemical Engineering Department, UDCT, Mumbai from 2003 to 2008. He was an Assistant Professor at Chemical Engineering Department, ICT, Mumbai from 2008 to 2011. He did his B.Tech. and M.Tech. from LIT, Nagpur and Ph.D. (Tech) from UDCT on 2006. He is a life member of IICHE (Indian Institute of Chemical Engineer), CSI (Catalysis Society of India), OTA (Oil Technologist Association), UAA (UDCT Alumina Association). He has controlled Major Administrative Position like Controller of Examinations of ICT Mumbai from 2018 to 2020. He was a Head of Training and placement cell of ICT from 2014 to 2019. He was a Headwarden of ICT Hostel, Mumbai from 2016-2018. He has got some prestigious awards like – Fellow Maharashtra Academia Sciences, Best Professor contributing in Research award by C. B. Murarka Charitable Trust, Hindustan

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Lever Biennial Award for the Most Outstanding Chemical Engineer of the year (2015), Outstanding Professor of ICT" award sponsored ISCMA. He has handled some Govt. sponsored Projects like-AICTE, IGCAR, DAE, DST, UGC, RGSTC. He has worked as Industrial Consultation and Technical consultant to various private companies. His Research Interests are – Catalysis, Wastewater treatment, Enzyme catalyzed Reactions (Bio-catalysis); Bio-diesel production and purification; Enzyme modification and purification, Process intensification using modern tools like ultrasound and microwave, Extraction of natural products; Multiphase reactor, Advance separation Processes (liquid-liquid extraction, crystallization, adsorption), Nanoparticles synthesis and its applications, utilization of waste for valuable products. He has guided total 101 M.Tech. students, 30 Ph.D. students and 6 postdoctoral students. Currently is involving for the guidance of 20 Ph.D. students, 13 M.Tech. students and 4 postdoctoral students. He has published 220 international journal articles with h-index 43 and citation > 6580. He now has total 7 private project and 3 government project. He has participated in 50 conferences/symposium. He has delivered 25 national and 6 international invited lectures. He has publisided a total 14 book chapters and 3 patents.

Carbon dioxide utilization to value added products

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The use of mono/bimetallic heterogeneous catalysts played important role in the conversion of platform molecules from biomass to various value-added products. The development of such catalysts is important as they offer the potential of increased activity and selectivity combined with enhanced stability as compared to their monometallic counterparts. Recently, we have reviewed the role of acid-functionalized catalyst for the synthesis of levulinate esters¹. We would like to present our recent work on various bimetallic catalysts like Co-Al, Ru-Mq-Al-Si, Ru-ZrO₂MCM-41 and Ru@GOIL. These catalysts were tested for the synthesis 2,5diformylfuran, 2,5-dimethylfuran, pyrrolidone from biomass derived substrates. In the first case study we have studied one pot conversion of fructose to diformylfuran using Co-Al hydrotalcites. The catalytic properties of the prepared Co-Al hydrotalcites in different molar ratio were investigated for the dehydration of fructose to 5-hydroxymethylfurfural (HMF), and then selective oxidation of the HMF into 2,5-diformylfuran (DFF) was studied². Next, synthesis of Ru metal supported on Mg-Al-Si was prepared and characterized by different characterization techniques. The catalytic effect of the prepared Ru-MMT in varied wt% of Ru metal were discovered for dehydration reaction of fructose to HMF, and for efficient oxidation of the HMF into DFF. Practical applicability of the developed catalyst was successfully demonstrated for direct transformation of various carbohydrates (glucose, inulin, sucrose, starch, raffinose and maltose) to DFF in moderate to good yield (35-64% yield). In another work we have developed effective catalytic route for the selective hydrogenolysis of HMF to high quality bio fuel 2,5-dimethylfuran (DMF) by using Ru supported on ZrO₂-MCM-41³. With the use of 2 wt% Ru ZrO₂-MCM-41 catalyst, 90% yield of DMF was obtained from HMF with very short reaction time of 1 h. The catalyst was recycled up to six time with marginal decrease in the yield after 4th cycle. Moreover, synthesis of ruthenium ion supported on ionic liquid immobilized into graphene oxide (Ru@GOIL) catalyst and characterized using different analytical techniques. The catalyst is highly active for the synthesis of N-aryl/alkyl pyrrolidones derivatives by reductive amination reaction and afforded products in 78–93% yield⁴. The catalyst was recycled for six reaction runs with slight drop-in activity after 4th cycle. Practical applicability of the developed catalyst was successfully demonstrated by

direct transformation of biomass waste (rice husk and wheat straw) derived LA to N-substituted pyrrolidones. We have also achieved one-step transformation of fructose to 2,5-diformylfuran over Ru metal supported on montmorillonite catalyst. In this case the catalyst showed promising results on the dehydration reaction of fructose to 5-hydroxymethylfurfural (HMF), and for the efficient oxidation of HMF into 2,5-diformylfuran (DFF)⁵. The ruthenium-catalyzed asymmetric transfer hydrogenation (ATH) of levulinic acid (LA) to chiral γ -valerolactone (GVL) was also demonstrated for the first time. ATH of LA has been explored with Noyori's chiral catalyst (Ru-TsDPEN) in methanol solvent⁶.

References

- 1. K. C. Badgujar, V. C. Badgujar and B. M. Bhanage, Fuel Processing Technology, 2020, 197, 106213.
- 2. A. B. Raut and B. M. Bhanage, ChemistrySelect, 2018, 3, 11388.
- 3. A. B. Raut, B. Nanda, K. M. Parida and B. M. Bhanage, Chemistry Select, 2019, 4, 6080.
- 4. A. B. Raut, V. S. Shende, T. Sasaki and B. M. Bhanage, Journal of Catalysis, 2020, 383, 206.
- 5. A. B. Raut, V. S. Shende and B. M. Bhanage, *New Journal of Chemistry*, 2020, 44, 13659.
- 6. V. S. Shende, A. B. Raut, P. Raghav, A. A. Kelkar and B. M. Bhanage, ACS Omega, 2020, 4, 19491.

Brief Bio-Sketch

Prof. Bhalchandra M. Bhanage obtained his doctorate from Pune University in 1996. He spent more than one year at Tohoku University, Japan (1997-1998) as a JSPS Fellow, and four years at Hokkaido University, Japan (2000-2003) as a CREST-JST fellow with Prof. M. Arai. In 2004, he joined the Institute of Chemical Technology, Mumbai, India as Professor of Industrial and Engineering Chemistry. Among his current interests is catalysis using CO₂, CO and H₂. He has worked on developing novel catalysts for various coupling reactions, carbonylation reactions, lonic Liquids (ILs) catalysis, hydroformylation reactions, amination reactions, etc. He is also working on nanomaterials synthesis, enzymatic catalysis, electrocatalysis, nanocatalysis, C-H bond activation and the use of non-conventional techniques like ultrasound and microwaves for various catalytic reactions. He has received more than 15000 citations with an h-index of 57. He is a Fellow of Maharashtra Academy of Sciences (FMASc) and the fellow of the Royal Society of Chemistry, and Fellow of the Biotech Research Society of the India.

Invention of new reactions for the synthesis of indole and carbazole based alkaloids

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More than 40% of the marketed drugs are derived from natural products and about 80% of the natural product derived drugs required synthetic efforts due to the scarcity in their availability. In addition, natural products play a pivotal role as the guiding principle behind synthetic drug designing and development. Synthesis of complex natural products, drugs, medicinally important compounds and organic-materials are heavily reliant on the availability



Scheme 1. Functionalizations of indole and pyrrole.

of sustainable reaction methods. Designing a new reaction often allow the synthesis of much complex molecules in a rather simpler way and also reduces both cost and efforts. In my independent research career from IIT Kharagpur, the syntheses of over 30 complex natural products of medicinal importance were accomplished in fewer synthetic steps by inventing novel reaction methods. The organo-catalytic alkenylation, alkylation, cationic cyclization reactions of indoles enabled synthesis of those alkaloids. Use of simple and cost-effective catalysts, easy reaction set-up and cheap starting materials are major highlights and render these methods sustainable for large scale application.

References

(a) S. Sahu, A. Banerjee and M. S. Maji, *Org. Lett.*, 2017, **19**, 464; (b) A. Banerjee, S. Sahu and M. S. Maji, *Adv. Synth. Catal.*, 2017, **359**, 1860; (c) S. Sahu, B. Das and M. S. Maji, *Org. Lett.*, 2018, **20**, 6485; (d) S. Saha, A. Banerjee and M. S. Maji, *Org. Lett.*, 2018, **20**, 6920; (e) M. R. Sk, S. S. Bera and M. S. Maji, *Org. Lett.*, 2018, **20**, 134; (f) S. S. Bera, M. R. Sk and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 1806; (g) A. Banerjee and M. S. Maji, *Chem. Eur. J.*, 2019, **25**, 11521.

Brief Bio-Sketch

Dr. Modhu Sudan Maji, is an Associate Professor at Department of ChemistryIndian Institute of Technology Kharagpur. He was a postdoctoral fellow at RWTH Aachen University, Germany under the supervision of Prof. Martin Oestreich from March 2010 to April 2013 with Alexander von Humboldt Fellow. Then he did his second postdoctoral research at Technical University Berlin, Germany under the supervision of Prof. Martin Oestreich from May 2013 to Novenber 2013. He did his Ph.D. under the supervision of Prof. Armido Studer, University of Muenster, Germany on 2009. He did his M.Sc. from Indian Institute of Science, Bangalore, India on 2006. He did his B.Sc. from University of Calcutta, Kolkata, India on 2003. He has published total 38 journal articles, and he has supervised 2 M.Sc. projects and has got 17 Awards/Honours/Membership. His research interest is on the field of Catalysis, Asymmetric Synthesis, Organometallic Chemistry, Natural Products Synthesis.

Caged phosphines: Controlling metal electronics for the exploration of novel synthetic pathways

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Phosphines as activating ligands have, in combination with transition metals, played an important role in the development of sustainable catalytic solutions for academia as well as industrial applications. Caged phosphines are a class of phosphines possessing threedimensional scaffolds and capable of providing unique control over steric and electronic properties. The versatility of the caged phosphine ligands has been demonstrated elegantly by the groups of Verkade, Gonzalvi as well as Stradiotto¹. Our contribution to this area comes in the form of the 1,3,5-triaza-7-phosphaadamantane-based caged ligands, especially PTABS (KapdiPhos) that has proved to be a revelation in promoting heteroarene functionalization in a highly efficient way. The talk will therefore be centered around the journey from the development of the ligand to the varied applications including scale-up possibilities, eventually culminating into its commercialization². Novel synthetic pathways



have also been explored due to the ease of control of electronics on the metal using the caged ligand.

References and Notes

- 1. M. Zablocka, A. Hameau, A.-M. Caminade and J.-P. Majoral, Adv. Synth. Catal., 2010, 352, 14.
- (a) V. Gayakhe, A. V. Ardhapure, A. R. Kapdi, Y. S. Sanghvi, J. L. Serrano, L. Garcia, J. Perez, J. Garcia, C. Fischer and C. Schulzke, *J. Org. Chem.*, 2016, **81**, 2713; (b) S. Murthy Bandaru, S. Bhilare, N. Chryosochos, V. Gayakhe, I. Trentin, C. Schulzke and A. R. Kapdi, *Org. Lett.*, 2018, **20**, 473; (c) S. Bhilare, S. Muthry Bandaru, J. Shah, N. Chrysochos, C. Schulzke, Y. S. Sanghvi and A. R. Kapdi, *J. Org. Chem.*, 2018, **83**, 13088; (d) H. Shet, U. Parmar, S. Bhilare and A. R. Kapdi, *Org. Chem. Front.*, 2021, **8**, 1599; (e) H. Shet, S. Bhilare, Y. S. Sanghvi and A. R. Kapdi, *Molecules*, 2020, **25**, 1645.

Brief Bio-Sketch

Dr. Anant R. Kapdi is UGC-Appointed Assistant Professor of Chemistry & Chief Central Training and Placement Coordinator (ICT Mumbai). He is a former Founding Deputy Director of ICT-IOC, Bhubaneswar (On deputation from ICT Mumbai) and Founding Coordinator (India) for The Innovation Sustainability Chemistry Consortium (ISCC). He was an Alexander von Humboldt Fellow with Prof. Lutz Ackermann, Goettingen University, Germany. He did his Ph.D. in Organic Chemistry, University of York, United Kingdom under the supervision of Prof. Ian Fairlamb and Co-supervision of Prof. Richard Taylor. He has got a number of awards and recognitions. He was a Fellow of Royal Society of Chemistry, London as Leaders in the Field category, 2021. He was an Invited Professor at University de Orleans, France in May 2019. He has got C. B. Murarka best Assistant Professor award on 2019. He was an Associate Editor of RSC Advances: Royal Society of Chemistry journal. He was a Fellow of Maharashtra Academy of Sciences on 2016. He got the DAAD Fellowship for Scientists. He got the DST-SERC Fast Track Fellowship for Young Scientists. He has published total 109 journal articles with highest impact factor of 54. He has edited 4 books of Book series on Palladium-Catalyzed Processes by Elsevier.

Discovery of novel synthetic methodologies for pharmaceuticals

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The discovery of *in situ* generated novel reactive species and their applications in cascade reactions to furnish the chiral/achiral drug-like molecules and pharmaceuticals will be discussed.



Scheme. Discovery of novel catalytic reactions for pharmaceuticals and agrochemicals.

References and Notes

- 1. P. Swamy, Md. A. Pasha, G. Thirupathi and D. B. Ramachary, Chem. Eur. J., 2019, 25, 14036.
- 2. A. Suresh Kumar, G. Thirupathi, G. S. Reddy and D. B. Ramachary, *Chem. Eur. J.*, 2019, 25, 1177.
- 3. D. B. Ramachary, Md. A. Pasha and G. Thirupathi, Angew. Chem. Int. Ed., 2017, 56, 12930.
- 4. D. B. Ramachary, A. B. Shashank and S. Karthick, *Angew. Chem. Int. Ed.*, 2014, 53, 10420.
- 5. D. B. Ramachary and M. Kishor, J. Org. Chem., 2007, 72, 5056.

Ramachary graduated with M.Sc. degree in School of Chemistry from University of Hyderabad and obtained Ph.D. in synthetic organic chemistry from Indian Institute of Science, Bangalore in 2001. He subsequently held postdoctoral position at the Scripps Research Institute for Catalysis, prior to joining University of Hyderabad in January 2005. He is a recipient of many awards including Fellow of the National Academy of Sciences, Allahabad-2021, Fellow of the Royal Society of Chemistry, London-2020 and Fellow of Indian Academy of Sciences, Bangalore-2018. He has guided 17-Ph.D. students and out of them, 4-Ph.D.'s got Eli Lilly & Company Asia Outstanding Thesis Awards 2011, 2012, 2013 and 2014. He is an Editorial Advisory Board Member, Organic & Biomolecular Chemistry, RSC Journal 2013-present, and Editorial Advisory Board Member, European Journal of Organic Chemistry, Wiley Journal 2017-present. Prof. Ramachary published more than 100 papers in both national and international reputed journals, two books on emerging organocatalysis area and few chemical reactions are named after him. Prof. Ramachary delivered more than 100 lectures in both national and international conferences.

Therapeutic and diagnostic nanostructures through self assembly

P. A. Hassan

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Self assembly of small molecules into complex hierarchical structures via non-covalent interactions offers an attractive route to design novel materials. Nanostructured materials formed by the self assembly of polymers, lipids or surfactants have attracted a great deal of attention in biotechnology, pharmaceutical and cosmetic industries. This lecture will address the role of intermolecular interactions in modulating the microstructure of self-assembled materials and its applications in creating functional nanostructures. In particular, we demonstrated a strategy to make surface functionalized nanostructures through self assembly of amphiphilic or small molecules for therapeutic purposes. Therapeutic and diagnostic applications of peptide functionalized magnetic nanoparticles will be discussed. Stimuli sensitive assemblies that can reversibly associate or dissociate in response to environmental changes have been fabricated, as a model system for self regulated drug delivery vehicle. A new phenomenon of self assembly in room temperature supercooled solvents and its applications will be discussed. The present findings have important implications in designing stimuli sensitive drug delivery systems.

Brief Bio-Sketch

Dr. P. A. Hassan joined Bhabha Atomic Research Centre (BARC), Mumbai in 1993 and presently serving as Head, Nanotherapeutics and Biosensors Section, Chemistry Division, BARC. He was a visiting researcher at the University of Louis Pasteur, Strasbourg, France in 1995. He pursued his post-doctoral research at the Department of Chemical Engineering, University of Delaware, USA in 2000-2002. He has visited advanced neutron scattering facilities like National Centre for Neutron Research, NIST, Maryland, USA and Institute Lau Langevin, Grenoble, France. He has co-authored more than 140 papers in peer-reviewed journals with a total citation of 6000 and h-index 42 (google scholar). His current research interests include microstructure and dynamics of self assembly, polymers, polyelectrolyte-surfactant interactions and nano drug delivery systems. He is an elected fellow of the National Academy of Sciences, India.

Biological applications of metal complexes and metal based nanoclusters





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In the first part of my talk, I will discuss about the rational design of metal complexes with potent anticancer activities¹. I will give a brief overview about the prodrug strategy that we have adopted to reduce the systemic toxicities and improve the selectivity^{2,3}. We used light as stimuli to convert the prodrug in to cytotoxic drug with high spatial and temporal control. This strategy is known as photoactivated chemotherapy (PACT), which is superior to the classical photodynamic therapy (PDT). Classical PDT relies upon oxygen for its activity, but under hypoxic (lack of oxygen) conditions observed in most of the tumor cells alleviate PDT activity, whereas PACT doesn't require oxygen for their anticancer activity making it as one of the promising cancer treatment modalities. In the second part of my talk, I will discuss about the design strategies of luminescent metal nanocluster for bioimaging and theranostic applications. In the area of metal nanoclusters, the syntheses and applications of copper nanoclusters are less extensively studied due to their facile oxidation and low redox potential (E° = 0.34 V)⁴. We have designed copper nanoclusters (CuNCs) with aggregation induced emission (AIE) characteristics, which provide extra stability and bright luminescence after aggregation⁵. Before conclude my talk, I will also discuss about our recent efforts to explore the applications of these stable AIE CuNCs in biology.

References

- 1. V. Venkatesh and Peter J. Sadler, *Met. Ions Life Sci.*, 2018, 18, 69.
- V. Venkatesh, C. J. Wedge, I. R. Canelón, A. Habtemariam and P. J. Sadler, *Dalton Trans.*, 2016, 45, 13034.
- 3. V. Venkatesh, N. K. Mishra, I. R. Caneloin, R. R. Vernooij, H. Shi, J. P. C. Coverdale, A. Habtemariam, S. Verma and P. J. Sadler, *J. Am. Chem. Soc.*, 2017, **139**, 5656.
- 4. A. Ganguly, I. Chakraborty, T. Udayabhaskararao and T. Pradeep, *J. Nanopart Res.*, 2013, **15**, 1522.
- 5. K. T. Prakash, N. Singh and V. Venkatesh, Chem. Commun., 2019, 55, 322.

Dr. Venkatesh V. is an Assistant Professor at Department of Chemistry, Indian Institute of Technology Roorkee from 2019. Before that he was a DST-INSPIRE faculty of Inorganic and Physical Chemistry (IPC) at Indian Institute of Science, Bangalore from April 2017 to 2019. He was a Post-Doctoral Fellow under the supervision of Professor Peter J. Sadler at Department of Chemistry, University of Warwick, UK from 2015 to 2017. He did his Ph.D. under the supervision of Professor Sandeep Verma at Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur, India from 2009 to 2014. He did his graduate course from Department of Chemistry, IIT, Kanpur, India on 2009. He did his M.Sc. from Anna University, India from 2006 to 2008 and B.Sc. from Gobi Arts and Science College, India from 2003 to 2006. He has got DST-INSPIRE faculty award from DST from April 2017. He has jointly awarded the Newton International Fellowship by Government of India from 2015 to 2017. He has got Eli Lilly and Company Asia Outstanding Thesis Award on 2014 from The Royal Society and The British Academy. Before that he was a senior research fellow from 2011 to 2014 and junior research fellow from 2009 to 2011 at Indian Institute of Technology-Kanpur, India. He had passed the NET examination on 2008. He has published about 21 papers and one book. He has 4 students working under his supervision for Ph.D. degree.

Catalytic mechanism of CO oxidation over zeolite supported Pd₄ cluster using QM/MM method



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Density functional theory calculation at PBE/DNP level shows an enhanced catalytic activity of CO + O₂ reaction catalysed by Pd₄ cluster. The rate-limiting step in this reaction is the dissociation of O₂ molecule on neutral Pd₄ cluster. When the Pd₄ cluster is supported on faujasite zeolite, the catalytic activity is found to enhance. Both Eley-Rideal (ER) and Langmuir-Hinshelwood (LH) mechanisms are invested for the reaction between CO and O₂. The CO oxidation takes place via both Eley-Rideal mechanism and Langmuir-Hinshelwood mechanisms. Since the energy barrier for ER mechanism in the gas phase calculation is lower than that for LH mechanism, we performed only ER mechanism in the supported Pd₄ cluster.

Brief Bio-Sketch

Prof. Deka has been working on fundamental aspects of catalysis, nanotechnology, drug design and atmospheric chemistry. He also carries out theoretical and experimental studies on heterogeneous catalysis with an aim to understand the nature of active sites and reaction mechanisms. He performs *ab initio* and density functional theory calculations to study electronic structure and reactivity of zeolite catalysts, metal clusters, supported metal clusters, carbon nanotubes, functionalized carbon nanotubes, varieties of drug molecules and volatile organic compounds. Prof. Deka's theoretical studies involve usages of new computational chemistry methodologies and expanding the scale and efficiency to provide realistic simulations. Prof. Deka also performs experimental studies in modifying zeolite, metal oxide nanoparticles and layered double hydrotalcite and uses them for various organic reactions. Professor Deka has published more than 200 research papers in international journals and 16 students got Ph.D. under his guidence.

Exploration of greener polybenzoxazines to unconventional applications





In the backdrop of rapidly depleting petroleum sources, it has become imperative to modify both the synthetic methodology and building blocks of polymers in accordance with the tenets of green chemistry. Nearly 90% of monomers and raw materials used in polymers industry are sourced from petroleum industries. However, both their origin and escalating non-biodegradable wastes has reached a plateau and demands the society for alternative solutions. Phenolic resins, the most widely used thermoset resin have certain limitations such as poor shelf life of the precursors, requirement of catalyst for polymerization, evolution of volatiles and volumetric shrinkage during cure etc. Polybenzoxazines (PBzs) is a class of addition cure resins has gained prominence as an alternative to conventional phenol formaldehyde (PF) resins. PBzs emerged as an altogether a superior class of polymers which may be attributed to a diverse set of properties ranging from high thermal stability and char yield, appreciable glass transition temperature, superior mechanical properties, low water absorption, near zero volumetric shrinkage, versatile molecular design flexibility, facile synthesis etc. There is a wide scope of applications viz. adhesives, composites, coatings, packaging etc. validating further exploration in this field.

Our research work involves synthesis and utility of bio-based benzoxazines for variety of applications keeping in view of green chemistry principles. My talk will encompass these efforts and will also discuss modulation of such compounds in novel unexplored applications such as energy storage devices to self-healants.

Bimlesh Lochab obtained an M.Sc. (1997-1999), M.Tech. (1999-2000) from IIT, Delhi, India and D.Phil. (2002-2005) from the University of Oxford and PDF at the University of Oxford and University of Nottingham, UK. Recipient of the Young Scientist Award 2009 to research on cardanol, a cashew-nut industry waste, sourced polymers. She joined, Shiv Nadar University (SNU), UP, in 2012 and now working as an Associate Professor in Department of Chemistry. She is a recipient of several research grants, awarded as the first Most Creative Research Award in 4th International Symposium on Polybenzoxazines, Luxembourg Institute of Science and Technology (LIST), June 2021, Research Excellence Award, Shiv Nadar University, 2021, selected by Chemical Research Society of India for CRSI Bronze award 2021 for outstanding achievements in the field of 'Materials Science'. Her pioneering work on Green Chemistry more specifically inverse vulcanization copolymers for Li-S battery application cited in several newspapers (PTI, 24th August 2020). She has been invited as an expert for a recording programme on "लीथियम ऑयन बैटरी" for Panel discussion, Vigyan Prasar, Department of Science and Technology, Govt. of India, 24th October 2019. Her several videos are available on YouTube. She is recently awarded for outstanding achievements "Distinguished alumna award 2020", Maitreyi College, University of Delhi, 16th June 2020. She has been invited several times for presiding sessions in ACS conferences and also invited to give first Lecture in the Young Talents and Upcoming Investigators, "The Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry". auspices of The Division of Polymeric Materials Science and Engineering (PMSE). She is a scholarship holder throughout her career, Young Scientist Award (DST, 2009-2013), Fellowship from C. R. Barber Trust Fund (IoP, UK, 2005), Felix Scholarship (UK, 2002-2005), Council of Scientific and Industrial Research-Junior Research Fellowship (1999-2000), Radha Sai Ram Memorial prize (1995). Membership of ACS (since 2013), APA (Lifetime), CRSI (Lifetime) and the Society for Polymer Science (India) SPS (Lifetime), Member of Institute of Physics (IoP, 2005-2006), Member of Polymer Physics group, (2005-2006). She is Chief Executive member of Sustainability Forum and National Advisory Committee Member in Asian Polymer Association (APA), 2020. Her research interests include Green and sustainable chemistry, Polymer architectures for PVs and OLEDs, Nanomaterials and their derivatives synthesis for Device applications (energy storage devices), Drug delivery applications Antibacterial applications. She has 4 patents and published 45 articles, 1 book and 4 book chapters.

Harnessing solar energy for fuel from water using carbon nitrides



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Although solar energy is abundant, harnessing in a proper way to leverage it is a formidable challenge. Making hydrogen, a green fuel (no carbon footprint) with high energy density, from water splitting is one of the stimulating research areas. The development of efficient metal-free photocatalyst from ample and sustainable precursors, which operates with visible light continues to be challenging in this field. The polymeric carbon nitride semiconductor, has recently attracted significant attention because it exhibits robust photocatalytic activity under solar irradiation¹. Crystallinity has strong impact on modulating the gears that involve in this surface photoredox reaction. In my presentation, I will delineate the development of crystalline carbon nitride and its photocatalytic activity under visible light. How the variation of carbon-nitrogen ratio changes the band gap and band position, thereby enhancing the visible light harvesting will be demonstrated². The trade-offs between crystallinity and light harvesting and their consequence on catalytic activity will be discussed. Moreover, the effect of cocatalyst size and its interface on the photocatalytic performance will be unveiled based on experimental results in conjunction with density functional theory^{3,4}.

References

- 1. X. C. Wang, K. Maeda, A. Thomas, K. Takanabe, G. Xin, J. M. Carlsson, K. Domen and M. Antonietti, *Nat. Mater.*, 2009, **8**, 76.
- 2. M. K. Bhunia, K. Yamauchi and K. Takanabe, Angew. Chem., Int. Ed., 2014, 53, 11001.
- 3. M. K. Bhunia, S. Melissen, M. R. Parida, P. Sarawade, J.-M. Basset, D. H. Anjum, O. F. Mohammed, P. Sautet, T. Le Bahers and K. Takanabe, *Chem. Mater.*, 2015, *27*(24), 8237.
- M. K. Bhunia, E. Abou-Hamad, D. H. Anjum, A. Gurinov and K. Takanabe, *Part. Part. Syst. Charact.*, 2017, 1700183. (Special Issue: Artificial Photosynthesis – Mimicking Nature for Renewable Energy Production).

Dr. Manas K. Bhunia is a specially appointed Assistant Professor at the WRHI and Materials and Structures Laboratory in Tokyo Institute of Technology. After receiving his Ph.D. (Supervisor: Prof. Asim Bhaumik) at Indian Association for the Cultivation of Science (IACS), India in 2012, he moved to USA to pursue postdoctoral studies under Prof. Alexandra Navrotsky at University of California, Davis. In 2013, he started another postdoctoral research with Prof. Kazuhiro Takanabe at KAUST Catalysis Center, KSA. Since July, 2017 to December, 2018, he worked as an Assistant Professor on contract at Central University of Tamil Nadu, India. His current research interest lies in understanding the role of surface and interface effect in heterogeneous catalysis with special emphasis on nanocluster catalysts.

Aliphatic processable functional porous polymers: Hierarchical synthesis via colloidal templating and application towards removal of pollutants



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Porous polymers established itself as one of the emerging material of interest for different applications, such as adsorbent materials, energy storage materials, catalysis etc.¹. Compared to its counterparts (MOF and COF), amorphous polymers have certain advantages, such as high thermal stability, better processability (expected for a polymer) etc. This inspires scientists over globe to prepare porous polymers using different approaches. Almost all porous polymers reported till date is based on polyaromatic frameworks, or copolymers of polystyrene – where the aromatic moieties took very significant role to generate (micro)porosity within the network^{2,3}. Porous polymers with complete aliphatic structures are rarely reported. This greatly



limits the scope of functional porous polymers – as large number of potential functional network structures don't exist. Moreover processability of porous polymers is another important issue in the current stage and need further attention. To address these issues we aim to prepare aliphatic processable functional porous polymers, with active functionalities such as amines and amides, via colloidal template approach where – hyperbranched polymer colloids were used as intermediate structures to develop such porous polymers in a hierarchical way. The microporosity was introduced via polymerization induced phase separation process – either via hydrophobic repulsion⁴ or via cationic repulsion⁵ of the growing hyperbranched polymer. The resultant porous polyamiono-amides show excellent ability to adsorb different pollutants, such as iodine, dyes and CO_2 . Moreover, choice of suitable hydrophilic network enable easy biodedradation in water.

References

- 1. B. Zheng, X. Lin, X. Zhang, D. Wu and K. Matyjaszewski, *Advanced Functional Materials*, 2020, **30**, 1907006.
- 2. D. Wu, F. Xu, B. Sun, R. Fu, H. He and K. Matyjaszewski, *Chemical Reviews*, 2012, 112, 3959.
- J. Wu, F. Xu, S. Li, P. Ma, X. Zhang, Q. Liu, R. Fu and D. Wu, *Advanced Materials*, 2019, 31, 1802922.
- 4. M. Avais and S. Chattopadhyay, ACS Applied Polymer Materials, 2021, 3, 789.
- 5. M. Avais, S. Kumari and S. Chattopadhyay, Soft Matter, 2021. doi: 10.1039/D1SM00441G Aliphatic.

Brief Bio-Sketch

Dr. Subrata Chattopadhyay is an Assistant Professor at Department of Chemistry, Indian Institute of Technology Patna from January 2017. He is the Head of the Sophisticated Analytical Instrument Facility (SAIF), IIT Patna. Before joining the department, he was a postdoctoral researcher at Ghent University, Belgium, under the supervision of Prof. Dr. Filip Du Prez, from November 2014-December 2016. He was a Research Assistant at DWI - Leibniz Institute for Interactive Materials, RWTH Aachen University, Germany, under the supervision of Prof. Dr. Martin Moeller and Dr. Helmut Keul from November 2013-October 2014. He has completed his Ph.D. from RWTH Aachen University, Germany, under the supervision of Dr. H. Keul. He has completed his M.Sc. from Indian Institute of Technology Madras on 2009 and B.Sc. from Raghunathpur College, The University of Burdwan on 2007. His primary area of research is Functional Polymers and materials. He has published total 17 peer reviewed journal articles and one patent.

Metal-Ligand coordination in some multifunctional inorganic systems for biomedical applications

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Chemical tools are needed to discover new effective drugs for tackling multifaceted complex neurodegenerative diseases like Alzheimer's disease, cancer etc. This presentation will be focused on our efforts to develop new inorganic systems for tackling these diseases. Design, synthesis and biological investigation of complexes containing analogous metal with similar or better activity compared to cisplatin towards cancer, has become an engrossing area of recent research. Promising anti-proliferative activity and less toxic side effects have been observed for ruthenium and copper based complexes compared to platinum drugs. Detailed characterization as well as biological investigations on DNA binding, DNA nuclease activity along with the steady state fluorescence quenching, synchronous fluorescence studies has also been done to understand the interactions with BSA. *In vitro* cytotoxic analyses for against breast cancer (MCF-7) or lung cancer (A549) cell lines by MTT assay and the trend of activity will be presented.

In addition, metals have many important functions in biology but also responsible for few serious metal-induced diseases due to their imbalance. Disruption of these metal-peptide interactions using chemical agents holds considerable promise as a therapeutic strategy to combat this incurable disease. Recent efforts in studying the Aβ-metal interactions have focused on small molecules, multifunctional chelators (MFCs), which can interact with the more than one target. Combining these features will lead to elaborated series of interesting new multifunctinal compounds. Various new molecular frameworks are developed or being developed in our laboratory for this purpose. Presentation will be on exploring their synthesis, characterization, binding behaviour, metal chelation, acetylcholinesterase inhibition, antiaggregation potential etc.

References

1. T. A. Khan, et al., New J. Chem., 2020, 44, 239.

- 2. S. Jain, et al., Dalton Trans., 2020, 49, 4100.
- 3. S. Jain, et al., J. Inorg. Biochem., 2020, 210, 111174.
- 4. M. Rana, et al., RSC Adv., 2020, 10, 28827.
- 5. M. Rana, et al., Metallomics, 2019, 11, 64.
- 6. A. K. Sharma, et al., J. Am. Chem. Soc., 2017, 139(36), 12550.
- 7. A. K. Sharma, et al., J. Am. Chem. Soc., 2012, 134, 6625.
- 8. L. Sun, A. K. Sharma, et al., ACS Chem. Neurosci., 2020, 11, 2741.

Dr. Anuj Sharma received his Master of Science in Chemistry from Indian Institute of Technology, Roorkee, in the year 2004 and then Ph.D. from Indian Institute of Technology, Kanpur in 2009 with Prof. Rabindranath Mukherjee in the area of Coordination Chemistry with special emphasis on magneto-structural correlations and electronic properties of metal complexes of non-innocent ligands. After completing Ph.D., he joined as postdoctoral fellow atWashington University in St. Louis, USA, with Prof. Liviu M. Mirica till March 2014 where his research work made an significant impact in the ongoing Alzheimer's disease research directions.

Dr. Sharma joined Department of Chemistry, Central University of Rajasthan in March 2014, as DST-INSPIRE Faculty before he became a regular Assistant Professor in December 2016. His research interests lie in inorganic chemistry, medicinal chemistry, synthetic inorganic and organic chemistry, to develop new smart inorganic complexes for applications in bio-imaging, therapeutic for cancer and neurodegenerative diseases like Alzheimer's disease.

He has more than 40 publications in high impact factor international journals and also a US patent to his credit. He has received Best research presentation awards in international conference of coordination chemistry, DST-INSPIRE faculty award, SERB International travel support and several sponsored research projects worth more than 10 million INR to his credit.

Tailor-made food formulation through alternative approach: A state of art

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Biotransformation of agricultural products into food is more than an art in today's food processing techniques. Since, the basic requirement of nutrition via food is essential for the survival therefore, the processing technologies are getting utmost priority for retaining more and more naturally occurring nutrients that are getting lost during the conventional practices. With the advancement of the societies, several specialization and trades are getting developed. The food intake behavior has also found to be different depending upon the spatial and temporal variations. The major challenge lies with the food technologist to develop the new processing technologies which are able to retain nutritional quality. To address this issue the scientists and the techno crats are going for the development of novel alternative method so that in a single go, both the challenges can be addressed.

Moreover, nowadays tailor-made food formulations adopting green technologies have also gained importance. As a result, customized designer food formulations are one of the major areas of research for the present generation. In one hand, minimum uses of chemicals/ thermos-chemical processes and on the other hand application of enzymes in food processing is getting priorities, where they help to achieve the desired attributes such as colour, flavour, texture, taste, appearance along with retainment of important nutrients that encompasses enriched minimally process food production. In Microbial Biotechnology and Downstream Processing laboratory the scientists and the researchers are actively involved in food biotechnological research with the objective of attaining/retaining maximum nutrition in food through modern processing i.e. customized designer food formulation. A co-relation between health and nutrition/specific diseases will be covered through this lecture. The important application of AI-ML in modern food processing will also be discussed.

Prof. Rintu Banerjee, Head, Agricultural and Food Engineering Department & Center for Rural Development and Innovative Sustainable Technology, Ex-MNRE Chair Professor is acknowledged as one of the leading enzymologists working in the area of Food, Fermentation and Bioenergy. She has completed her Ph.D. from Biotechnology Unit, Chemical Engineering Department, IIT Kharagpur.

She was bestowed with the prestigious Rafi Ahmed Kidwai award, Panjabrao Deshmukh Outstanding Women Scientist Award, Louis Pasteur, Recognition-award, Best-Teacher, Women Bioscientist, and Fellow of different esteemed societies and academy.

Her significant contributions comprise of cost-effective industrial enzymes production using agroresidues with immense applications in food and biofuel industries. Prof. Banerjee has established a novel 2G ethanol technology with a bio-refinery concept which harmonizes circular economy.

Through her innovative research, she has been granted with 03 international and 08 national patents, of which 10 technologies have been transferred to different industries and agricultural stakeholders. Prof. Banerjee guided 39 Ph.D.s, published 204 articles, 48 book chapters, authored and edited a book entitled Environmental Biotechnology, Oxford University Press and OMICS based approaches in Plant Biotechnology, Wiley-Scrivener Publishing.

Toward open-shell polycyclic hydrocarbons

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Polycyclic hydrocarbons (PHs) have positioned themselves at an important crossroad of chemical research by drawing enormous attentions from the different fields of science. Some noteworthy examples are: (1) basic molecular orbital theory was developed with PHs as model test cases whose properties such as resonance energies could be readily varied by changing fusion modes of certain rings; (2) organic dye-stuff chemistry relies on combination of PH cores with various auxochromes; (3) search for PHs as carbon-containing materials in interstellar space is an intense research topic in astrophysics; (4) pentacene, made from linear fusion of 5 benzenoid rings, is regarded as a benchmark molecule for organic semiconductors; (5) benzo[a]pyrene is a PH which is metabolized by initial enzymatic epoxidation, and is known as a carcinogen that comes from cigarette smoke; (6) repeated angular fusion of benzene rings have produced new type of chirality in π -conjugated helicenes. Despite such potentially important aspects of PHs, majority of the research on PHs was limited to the toxicological analyses and synthetic method developments in organic chemistry. The last decade has witnessed a revival of the chemistry of PHs from the synthetic and functional perspectives, and in my talk, I shall be highlighting my group's recent efforts in the syntheses of tetraradicaloid non-alternant PH and diradicaloid nanographene.

Brief Bio-Sketch

Dr. Soumyajit Das is working as an Assistant Professor at the Department of Chemistry, IIT Ropar, since March 2019. He obtained his B.Sc. in Chemistry (Honours) from Bagati Sreegopal Banerjee College (under The University of Burdwan) in 2005, and moved to IIT Guwahati to pursue his M.Sc. in Chemistry. He joined Prof. Sanjio S. Zade's group in IISER Kolkata, in 2007, and worked on the area of conducting polymers comprising selenophene or thiophene rings. In 2012, Soumyajit joined the group of Prof. Jishan Wu at the National University of Singapore to work on new near-IR dyes and fully conjugated macrocycles. After completing his postdoctoral studies in Singapore, he returned to India on August 2016 and gained nearly two-and-half years of industrial experience in the area of medicinal chemistry (Sai Life Sciences (2016-2018), Aurigene (2018-2019)) before starting his independent research career at the IIT Ropar. His current research interest is focused on the chemistry of fused polycyclic arenes and heteroarenes, as potential organic spin-electronic materials.
Luminescent rare-earth based metal-organic phosphors: Synthesis, structure and chemical recognition properties



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Rare earth based metal-organic Phosphors (ReMOPs) have emerged as an interesting family of compounds for which new properties are increasingly being found. Based on the potential of ReMOPs for their optical properties, large numbers of investigation have been carried out during the last decade. Among these investigations, chemical recognition properties using their luminescence properties are increasingly becoming an attractive and useful topic of research¹.

Rare earth based MOP (ReMOP) are unique due to their sharp emission line, large stokes shifts, long lived emission and high quantum yield. Besides that, the luminescence property of rare earth ions is highly dependent on the structural details of the coordination environment around the metal ions and usually not quenched by the oxygen despite of its long lived excited lifetime which provides a unique power for the effective chemical recognition². Increasing demand for timely and accurate environmental pollution monitoring and control requires new chemicals recognition techniques with outstanding performance, i.e. high sensitivity, high selectivity, and reliability. Due to forbidden nature and weak oscillator strengths of f-f transitions, direct excitation of lanthanide into 4f excited levels is practically very small and produces low level of luminescence. To overcome this situation lanthanide ions require indirect excitation called "antenna effect" i.e. metal ion is excited through its surrounding ligands by energy/electron transfer process. The ligand get excited by the absorption of excitation light, and then the energy is transferred to the lanthanide ion through non-radiative process, and finally lanthanide ions emit its characteristic luminescence. This process gives a huge advantage, firstly, in terms of large stokes shift which facilitate the clear detection of lanthanide luminescence separately from its excitation light and the ligand centred luminescence⁴. Secondly, it provides many fold increase of luminescence quantum yield in normal condition at room temperature¹. In most cases lanthanide luminescence is phosphorescence in nature which in general is very weak in room temperature due to solvent

quenching and self quenching of the long lived excited state. In MOPs, as lanthanide ions are embedded through organic ligands, the chance of solvent quenching as well as self quenching has been almost nullified. As a result lanthanides in MOPs give so strong luminescence that it is even visible by naked eye³. This enhanced luminescence is the most important feature of the ReMOPs for the application towards chemical recognition.

ReMOPs can selectively recognise many chemicals (molecules, ions, bio-molecules etc.) with excellent efficiency¹. The sensitivity is exhibited by the quenching (turn-off) or enhancement (turn-on) of luminescence intensity. Luminescence quenching (or enhancement) means the decrease (or increase) of luminescence intensity of a sample due a molecular interaction between the MOP and chemical. Depending upon the nature of MOP and the chemical, quenching of luminescence intensity occurs due to many reasons which include ground state complex formation, collision among luminophore and analyte, and many excited state processes like Förster resonance energy transfer (FRET), photoinduced electron transfer (PET), intramolecular charge transfer (ICT), Metal-ligand charge transfer (MLCT), excited state proton transfer (ESPT) etc.^{5–9}.

Over the past decade scientists have utilized the luminescence property of the MOPs for the recognition of ions, molecules, pH and temperature¹. In this presentation, our recent research work based on synthesis, structure and chemicals recognition properties of ReMOPs would be described and discussed^{10–14}.

References

- 1. P. Mahata, S. K. Mondal, D. K. Singha and P. Majee, Dalton Trans., 2017, 46, 301.
- D. K. Singha, S. Bhattacharya, P. Majee, S. K. Mondal, M. Kumar and P. Mahata, *J. Mater. Chem. A*, 2014, 2, 20908.
- 3. D. K. Singha, P. Majee, S. K. Mondal and P. Mahata, Eur. J. Inorg. Chem., 2015, 1390.
- 4. D. K. Singha, P. Majee, S. K. Mondal and P. Mahata, *RSCAdv*, 2015, 5, 102076.
- 5. D. K. Singha and P. Mahata, *Inorg. Chem.*, 2015, **54**, 6373.
- 6. D. K. Singha, P. Majee, S. Mondal, S. K. Mondal and P. Mahata, *Inorg. Chem.*, 2018, 57, 12155.
- P. Daga, P. Manna, P. Majee, D. K. Singha, S. Hui, A. K. Ghosh, P. Mahata and S. K. Mondal, *Dalton Trans.*, 2021, 50, 7388.
- 8. P. Majee, D. K. Singha, P. Daga, S. Hui, P. Mahata and S. K. Mondal, *CrystEngComm.*, 2021, **23**, 4160.
- 9. P. Majee, D. K. Singha, S. K. Mondal and P. Mahata, *Photochem. Photobiol. Sci.*, 2019, 18, 1110.
- 10. D. K. Singha, P. Majee, S. K. Mondal and P. Mahata, Eur. J. Inorg. Chem., 2016, 4631.
- 11. S. Hui, P. Majee, D. K. Singha, P. Daga, S. K. Mondal and P. Mahata, *New J. Chem.*, 2021, **45**, 9394.
- 12. P. Daga, S. Sarkar, P. Majee, D. K. Singha, S. Hui, P. Mahata and S. K. Mondal, *Mater. Adv.*, 2021, **2**, 985.

- 13. P. Majee, P. Daga, D. K. Singha, D. Saha, P. Mahata and S. K. Mondal, *J. Photochem. Photobiol. A*, 2020, **402**, 112830.
- 14. D. K. Singha, P. Majee, S. Hui, S. K. Mondal and P. Mahata, *Dalton Trans.*, 2020, 49, 829.

Brief Bio-Sketch

Dr. Partha Mahata is an Assistant Professor of Inorganic Chemistry Section, Department of Chemistry, Jadavpur University since 2017. Before that, he was an Assistant Professor at Department of Chemistry, Suri Vidysagar College, Suri from 2015 to 2017. He was DST Inspired Faculty at S. N. Bose National Centre for Basic Sciences, Kolkata from 2013 to 2015. He was an Assistant Professor at School of Chemistry & Bio-Chemistry, Thapar University from 2012 to 2013. He did his postdoctoral research work in the field of Synthesis, Structure and Properties of Meso-Porous Crystalline Metal-Organic Coordination Networks at Department of Applied Chemistry, School of Engineering. The University of Tokyo from 2009 to 2011 under the guidance of Prof. Makoto Fujita. He did his Ph.D. in the field of Synthesis, structure, magnetic, photoluminescence and photocatalytic properties of metal-organic framework compounds Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India from 2003 to 2009 under the guidance of Prof. Srinivasan Natarajan. He had received several prestigious awards and fellowships. He has published total 70 research articles with total citation of 2750 and h-index is 27. His area of research is Metal-Organic Materials, Mixed Metal Oxides, Magnetic and Luminescent Materials, X-ray Crystallography.

Conceptual advances versus empirical approach in electrocatalysis



Sayan Bhattacharyya

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The energy conversion and storage systems of the 21st century heavily depend on the design of state-of-the-art electrocatalysts. The catalyst performance depends on several intrinsic factors such as electrochemically active surface, mass activity governing the reaction kinetics, electronic environment of the active sites, electrical conductivity etc. Since the adsorption and desorption of reaction intermediates occur on the surface of the electrocatalyst, major attention is focused on their design besides the substrate on which the catalyst is anchored. Many of these developments are based on empirical methods trying through several compositions from the periodic table of elements. Although new concepts are brought-in through such serendipitous achievements, the real challenge is to build on a research idea and move towards the goal. This lecture will discuss few case studies of such challenges and solutions towards hydrogen fuel and metal-air battery.

Brief Bio-Sketch

Sayan Bhattacharyya is the Professor of Department of Chemical Sciences and Centre for Advanced Functional Materials, IISER Kolkata. His current research interests are: (1) Electrochemistry; (2) Photovoltaics with metal-halide perovskite nanostructures; (3) Metal-air battery; (4) Photorechargeable battery. He is the Lifetime Fellow of the Indian Chemical Society, since 2020.

Nontraditional aliphatic light-emitting polymers for multipurpose applications: Structure, property, and performance relations



Nayan Ranjan Singha

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The development of intrinsically luminescent multifunctional macromolecules and understanding their fluorescence characteristics are highly desirable to broaden further the scope of nontraditional macromolecular luminogens. Nowadays, the intrinsically fluorescent (nontraditional) multifunctional polymers are of huge demand because of the diverse applications in sensing, superadsorption of organic and inorganic pollutants, monitoring plant signaling molecules, bioimaging, data encryption, energy storage, and devices. In this regard, the biocompatibility and the aggregation-enhanced emission (AEE), excitation-dependent emission (EDE), concentration-induced emission (CIE), and clustering-triggered emission (CTE) in multifunctional stimuli-responsive light-emitting polymers broaden further the performance potential and application prospects of these multifunctional nontraditional fluorescent macromolecules. Recently, we are working on the strategic synthesis of nontraditional multifunctional light-emitting co-, ter-, tetra-, and penta-polymers via multi C-C, O–C, and N–C coupled facile polymerization of nonfluorescent hydrophilic or hydrophobic monomers in water medium, in which third, fourth, or fifth co-monomer has been attached in situ during polymerization. Additionally, to get the heteroatomic subluminophores, extra branching, crosslinked structure, diverse functionalities, and enhanced fluorescence in the as-prepared intrinsically-fluorescent polymers, the highly-branched multifunctional natural polymer(s) have been grafted into co-, ter-, tetra-, or penta-polymers for developing the interpenetrating multipolymer networks. In addition, primary-, secondary-, and tertiary-amide based nontraditional blue, green, and red light emitting multifunctional polymers have been prepared, in which through space $n-\pi^*$ conjugation, N-branching, structural rigidity, intra- or inter-molecular hydrogen bonding, AEE, and CTE contributed cumulatively in the fluorescence properties of polymers suitable for selective and sensitive sensing along with the high-

performance exclusions of M(II/III) ions, high-contrast imaging of normal and cancer cells, security ink, and logic functioning. The contributions made by us will be helpful to the greater scientific community directly or indirectly involved in research works related to the diverse technologically important developments based on the nontraditional multifunctional light-emitting polymers.

Brief Bio-Sketch

Dr. Nayan Ranjan Singha is an Assistant Professor, WBGS, Department of Polymer Science and Technology, Government College of Engineering and Leather Technology (Post-Graduate), Maulana Abul Kalam Azad University of Technology, Block-LB-11, Salt Lake City, Kolkata, India. Dr. Nayan Ranjan Singha obtained Ph.D. from University of Calcutta in 2010 and underwent postdoctoral studies at University of Calcutta and Jadavpur University. Dr. Singha joined as a faculty of post-graduate division and started independent research career at Government College of Engineering and Leather Technology (Post-Graduate), Maulana Abul Kalam Azad University of Technology, Kolkata, India. Dr. Singha has been working on strategic synthesis of intrinsically fluorescent light-emitting polymers, nonconventional conducting macromolecules, and multifunctional stimuli-responsive hydrogels suitable for diverse applications, such as sensing, separation, bioimaging, device, and energy; synthesis of reactive functional polymers via RAFT, ATRP, ROP, PISA, emulsion, and solution polymerization; synthesis of nonconventional redox polymers for device applications; synthesis of metal-polymer frameworks (MPFs) for catalysis of organic reactions; intrinsically fluorescent macromolecules for sensing, detection, quantification, and separation of biologically active molecules; mimic of conventional solution-phase organic reactions in polymeric (solid) interfaces; nonconventional conducting polymers for energy and device application(s), modified graphene, or CNT based nanocomposites and membranes for sensing and separation; and computational analyses via DFT, TD-DFT, NTO, and RDG . Dr. Singha corresponded/published more than sixtyfive (65) research items including articles, reviews, and book chapters. Dr. Singha is the member of Indian Chemical Society (ICS/LM) Indian Institute of Chemical Engineers (IIChE/LM), American Chemical Society (ACS), Royal Chemical Society (RSC), and Forum of Scientists Engineers and Technologists (FOSET/ LM). Dr. Singha has completed two DST sponsored major research projects and has been working on major research project sponsored by CSIR (Government of India).

Theranostic applications of carbon nanomaterial modified sensors: A promising future



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The last few years have witnessed a substantial technological renaissance that boosted the development of nanomaterials which have a great impact on biosensing. The unprecedented properties of carbon nanotubes, fullerenes and graphene have catapulted carbon materials in the hotspot of biomedical research. Of particular interest is the integration of these materials into analytical systems that impact key research areas, in particular: medical diagnostics, multi-modal drug delivery, bio-imaging, environmental monitoring and biocatalytic sensing. Carbon nanomaterials offer unique advantages that span several domains, such as a high surface-to-volume ratio, high electrical conductivity, chemical stability, biocompatibility and robust mechanical strength. Thus, they are frequently incorporated as sensing elements.

The interface of electrochemistry and nanotechnology is a captivating playground for the elemental research and has eventually emerged as a futuristic and sustainable platform. Electrochemistry has always provided analytical techniques characterized by instrumental simplicity, moderate cost and portability. The innovative surface functionalizations by the integration of the carbon nanomaterials with nanoparticles, enzymes, DNA, polymers, ionic liquids, etc., would thereby augment the applicability of the sensors. Efforts have been made in our group to develop new-fangled approaches for the electrochemical detection of non-steroidal anti-inflammatory drug; antihypertensive agent, antiviral drug and natural alkaloid related to hepatocellular carcinoma. The proposed nanomaterial based sensors exhibited pronounced analytical performance and provided a new and powerful paradigm in terms of novel and augmented functionality that encompasses a wide variety of applications in clinical diagnostics and biological research. The developed electrochemical sensors comprised of novel nanomaterials had great potential for enhancing and superseding the capabilities of current molecular diagnostics by allowing rapid and highly accurate diagnoses, the integration of diagnostic and therapeutic capacities and the realization of personalized medicine.

Brief Bio-Sketch

Dr. Sanghamitra Chatterjee has published total 32 international publications, with total impact factor 249.532, citation 2305 (Scopus) and h-index 18 (Scopus). Her research interest lies in the field of organic electrochemistry, biomedical applications of nanomaterial modified sensors, development of sensors for biomolecules, drugs and doping agents, biosensors and arrays and electrochemical sensing techniques for clinical diagnostics and environmental monitoring. She is involved for the guidance of total 4 Ph.D. student at present time and 11 M.Sc. students have completed their project under her guidance. She is the member of many prestigious agency viz. member of American Chemical Society, life member of Society for Materials Chemistry, life member of Indian Society for Electroanalytical Chemistry and life member of Association of Chemistry Teachers. She has got several prestigious awards, certificate and fellowship. She had got 1st rank in Lucknow University in M.Sc. in 2005. She has incorporated in one review article and two book chapters. She did her post-doctorate work from Lakehead University, Ontario, Canada. She did her Ph.D. from Indian Institute of Technology (IIT), Roorkee, India. She completed her M.Sc. and B.Sc. degree from Lucknow University, Lucknow, India.

Optimisation of fire and gas detectors using 3D mapping technique



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Fire and Gas (F&G) detection system is one of the most crucial layers of protection in process industries. Successful F&G detection helps preventing escalation of small F&G events to potential catastrophic losses of life, asset, business, environment and reputation. Risk based approach provides important guidance in identifying plant areas where installation of F&G detection would bring best cost benefit and also on the executive actions that should follow after successful detection. However, an ALARP (As Low As Reasonably Practicable) risk can be achieved subject to proper optimization of the type & quantity of detectors, their locations, viewing angles vs the coverage target by means of 3D F&G detection mapping tools. This exercise takes into account several factors such as anticipated types of F&G leak events and associated risk, degree of plant congestion, ventilation, obstruction/shadows provided by equipment, piping and structural members, detection technologies vs potential spurious triggers, maximum utilisation of available supports and access for F&G detector maintenance etc. A high level guidance on the optimization technique using 3D mapping tool will be provided during this presentation based on hands on experience in this field.

Brief Bio-Sketch

Mr. Dipak K. Pahari is founder Director of NRGtech Services Pvt. Ltd. The latter is a leading multinational company in the fields of risk assessment and loss prevention engineering. Headquartered in Kolkata, NRGtech has successfully delivered over 90 projects around the globe during past 6 years of its existence. Mr. Pahari has 30 years of experience as a risk and reliability specialist for the process industries. Prior to establishing NRGtech, Mr. Pahari has gained extensive hands on experience in technical safety while serving major multinational clients during his tenure of 7 years with Engineers India Ltd. in New Delhi and 17 years with Technip in Abu Dhabi, Paris and Bangkok. He has chaired over 100 formal safety assessment workshops such as HAZOP, HAZID, ENVID, OHID, LOPA/SIL/IPF, PHSER, ISDR, HFE etc. He has conducted numerous training programs in Process Safety Engineering in India and abroad.

Sustainable catalytic conversion of waste plastic to virgin plastic

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India is generating significant plastic waste (~10 MMTPA), which is a cause of major environmental concern. However, if suitable technology is developed, this waste can produce ~8 MMTPA equivalent syncrude. Most of the processes used so far for plastic conversion are thermal in nature, thus having several unresolved challenges e.g. unstable liquid product, sticky char/tar formation, leakages between moving and stationary parts etc. Reliance R&D has developed a reliable and commercially viable process for efficient catalytic conversion of waste plastic. The process can convert unsegregated waste plastic to high yield of stable liquid product i.e. syncrude in presence of proprietary catalyst in a rotary reactor at lower temperatures than thermal route. Since catalytic, the process leads to high liquid yield (~80 wt%), low char yield (~5 wt%) with stable liquid product of high API (~35) having more gasoline and diesel range fractions and lower % of heavies. The process has been proved at a continuous pilot scale (~0.3 tpd) with different feed including mixed plastic waste, single use plastic and multi-layer plastic (MLP) etc. Efforts are on to scale up this further and commercialize it early. RIL has developed another path-breaking technology called MCC (Multizone Cat Cracking) which can convert the syncrude from plastic oil to high yield of polymer feedstock (70%). Thus the catalytic pyrolysis + MCC together can provide very high circularity of waste plastic to virgin plastic of ~ 55% via chemical recycling route. It is hoped that with fast commercialization of these innovative technologies, high circularity can be achieved in the polymer industry, thereby providing much needed sustainability in the plastic business.

Brief Bio-Sketch

Dr. Asit K. Das is currently Head of Refining R&D Centre in Reliance Jamnagar Refinery. He joined RIL in 2006 and established the Refinery R&D Centre at Jamnagar. Prior to that worked at Indian Oil R&D Centre since 1985. He is Ph.D. in Chemical Engineering with R&D experience over 35 years and has developed and commercialized many technologies e.g.Indmax, MCC, DSO, EPR etc. He has > 100 patent and > 80 publications with 7 book chapters to his credit. He has received many awards and recognition. He was the President of Engineering Science in the last Indian Science Congress in January 2020 at Bangalore.

Ligand-enabled oxidative gold catalysis

Nitin T. Patil



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The past two decades have remodelled the impression of gold from being an exorbitant glittery metal to the best catalyst for the activation and functionalization of various C–C multiple bonds. However, inspite of the reasonable efforts, the applicability of gold catalysis to the highly important cross-coupling reactions has remained highly limited. A prime reason for this is gold's reluctance to undergo the necessary oxidation state changes (Au: $E_0 = +1.41$ vs Pd: $E_0 = +0.92$ V) to catalyze cross-coupling reactions. With due credit to the pioneering work from the groups of Toste, Zhang, Hashmi and Glorius, two major strategies for achieving the inevitable Au(I)/Au(III) cycle have been developed which include: (a) external oxidant empowered Au(I)/Au(III) catalysis, (b) Au(I)/Au(III) catalysis via merged gold/photoredox strategy. Recently, our research group introduced an entirely new strategy wherein the use of benziodoxolones facilitates the Au(I)/Au(III) catalysis.



Scheme 1. Gold-catalyzed reactions via ligand-enabled Au(I)/Au(III) catalysis.

In this presentation, I will be discussing a new mode of harnessing Au(I)/Au(III) catalysis wherein an ancillary P,N-ligand lowers the activation barrier for the oxidative addition of aryl

halides to Au(I) and stabilizes the resulting Au(III)-aryl complex by P,N-coordination. The approach opens up new gateways for the development of enantioselective transformation by designing novel chiral P,N-ancillary ligands. Our explorations in the field of ligand-enabled Au(I)/Au(III) catalysis for achieving cross-coupling as well as 1,2-difunctionalization reactions of C–C multiple bond shall be discussed.

References and Notes

- Review: M. O. Akram, S. Banerjee, S. S. Saswade, V. Bedi and N. T. Patil, *Chem. Commun.*, 2018, 54, 11069.
- 2. (a) S. Banerjee and N. T. Patil, *Chem. Commun.*, 2017, **53**, 7937; (b) S. Banerjee, B. Senthilkumar and N. T. Patil, *Org. Lett.*, 2019, **21**, 180.
- (a) M. O. Akram, A. Das, I. Chakrabarty and N. T. Patil, *Org. Lett.*, 2019, **21**, 8101; (b) C. C. Chintawar, A. K. Yadav and N. T. Patil, *Angew. Chem. Int. Ed.*, 2020, **59**, 11808; (c) A. G. Tathe, C. C. Chintavar, V. W. Bhoyare and N. T. Patil, *Chem. Commun.*, 2020, **56**, 9304; (d) A. G. Urvashi Tathe, A. K. Yadav, C. C. Chintawar and N. T. Patil, *ACS Catal.*, 2021, **11**, 4576.

Brief Bio-Sketch

Dr. Nitin T. Patil is an Associate Professor of Department of Chemistry, IISER Bhopal. Before that, he was a Senior Scientist at Division of Organic Chemistry, CSIR-NCL, Pune from 2013 to 2017. He was a Senior Scientist at Organic Chemistry Division-II, CSIR-IICT, Hyderabad from 2011 to 2013. He was a QRS at Organic Chemistry Division-II, CSIR-IICT, Hyderabad from 2008 to 2011. He was a research fellow at The Scripps Research Institute, La Jolla, CA under Professor K. C. Nicolaou. From 01-2008 to 07-2008, he was a research fellow at Institute of Chemical and Engineering Sciences, Singapore under Professor K. C. Nicolaou from 2006 to 2007. He was an Assistant Professor at Department of Chemistry, Graduate School of Science, Tohoku University, Japan under Professor Yoshinori Yamamoto from 2005 to 2006. He was a JSPS Postdoctoral Fellow at Department of Chemistry, Graduate School of Science, Tohoku University, Japan under Professor Yoshinori Yamamoto from 2002 to 2005. He was a Postdoctoral Fellow at Institut für Organische Chemie, University of Goettingen, Germany under Professor Christoph Schneider from 03-2002 to 11-2002. From he did his Ph.D. from 1997 to 2002 from University of Pune, India. He did his M.Sc. and B.Sc. from North Maharashtra University, Jalgaon, India on 1997 and 1995 respectively. His broad research interests include development of metal-, organo- and organo/metal-catalyzed enantioselective methods and total synthesis of natural products. He has been the recipient of SERB Distinguished Investigator Award-2018, CRSI Bronze Medal-2018, INSA Young Scientist Medal-2010, Alkyl Amines-ICT Foundation Day Young Scientist Award-2010 and Avra Young Scientist Award-2012. He has also served as "Young Associate" of the Indian Academy of Sciences, Bangalore for the years 2010-2013. Recently, he was elected as a Fellow of The National Academy of Sciences (FNASc).

Oncogenic characterization of ATAD2 in stomach cancer



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The burden of stomach cancer incidence and death is a global challenge. Treating stomach cancer remains immensely difficult due to the lack of available markers to detect the disease at the early stages. Therefore, there is an immense demand for finding out an early detection biomarker for stomach cancer. Recently, ATAD2 is found to be overexpressed in stomach cancer with high prognostic significance and recognised as a promising biomarker for stomach cancer. ATAD2 is a unique cancer/testis antigen (CTA) that belongs to both AAA + ATPase and bromodomain family proteins. However, nothing much is known about the mechanism of ATAD2-mediated stomach carcinogenesis. Using bioinformatics analyses as well as studies with stomach cancer cells and stomach biopsy tissue samples, we address the regulation and function of ATAD2 expression in stomach cancer.

We show that ATAD2 is overexpressed in the most common intestinal type of stomach adenocarcinoma, and enhanced expression of ATAD2 is observed in all stages and grades of stomach cancer. Our immunofluorescence microscopy study with stomach biopsy tissues confirms the high expression of ATAD2 both in stomach adenocarcinoma and metastatic stomach tissue samples. Survival analysis indicates that upregulated ATAD2 expression drastically affects the survival of stomach cancer patients. Since *H. pylori* infection, and hypoxia are the major contributing factors for stomach carcinogenesis; we further study their role in ATAD2-mediated stomach malignancy. An enhanced expression of ATAD2 is observed in *H. pylori*-infected stomach cancer cells. We identify ATAD2 as a hypoxia-responsive and HIF1 α -regulated gene and elucidate that upregulated expression of ATAD2 enhances proliferation and migration of hypoxic stomach cancer cells. We further recognize the protein-protein interaction (PPI) network of ATAD2 with the top-ranked partners like ESR1 (or ER α), NCOA3 (or ACTR/SRC3/AIB1), SUMO2, HDA11 (HDAC11), SPTN2 (SPTBN2), and MYC. Among them, ESR1, MYC, NCOA3, and HDA11 are oncoproteins. Most strikingly, we report the participation of two druggable targets of ATAD2, i.e. AAA + ATPase and bromodomain in

the ATAD2-PPI network; ESR1, SUMO2, SPTN2, and MYC show a preference for bromodomain, whereas NCOA3 and HDA11 prefer ATPase domain of ATAD2. The importance of such findings in terms of targeting bromodomain-PPI and/or ATPase-PPI interfaces to curtail stomach cancer is elucidated.

References

- 1. A. Nayak, M. Dutta and A. Roychowdhury, *Life Sci.*, 2021, **9**, 119322.
- 2. A. Nayak, S. Kumar, S. P. Singh, A. Bhattacharyya, A. Dixit and A. Roychowdhury, *J. Biomol. Struct. Dyn.*, 2021, **13**, 1.
- 3. A. Nayak, A. D. Roy, N. Rout, S. P. Singh, A. Bhattacharyya and A. Roychowdhury, *Biochem. Biophys. Res. Commun.*, 2020, **523(4)**, 916.

Brief Bio-Sketch

Dr. Anasuya Roychowdhury, is an Assistant Professor of School of Basic Sciences (Chemistry and Biosciences) at Indian Institute of Technology Bhubaneswar, India. She did her Ph.D. at The University of Texas Medical Branch at Galveston, USA with Prof. Wlodek Bujalowski and postdoctoral research with Prof. Daniel Finley at Harvard Medical School, USA. Dr. Roychowdhury's current research focuses on cancer (gastrointestinal cancers) biology and therapeutics.

Laterite based indigenous arsenic removal technology: From the laboratory to the field

Sirshendu De



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Laterite is a locally available natural soil. It contains huge amount of iron and aluminum oxides and hydroxides that are potent adsorbent for arsenic removal. In this talk, it will be described how this naturally occurring abundant material is converted a low cost material for asenic removal and how that would be deployed to real life community scaled filters. The advantages, modeling, scaling up and the cost analysis of such a filter would be presented in this talk.

Brief Bio-Sketch

Prof. Sirshendu De did his B.Tech. (1990), M.Tech. (1993) and Ph.D. (1997) from Department of Chemical Engineering, IIT Kanpur. His main research interest includes membrane separation, membrane casting and various applications, process developments, modeling and design; flow modeling, heat and mass transfer in microchannel, mathematic modeling of different Chemical Engineering processes. He has authored 8 books, 15 patents, 318 publications in journals of repute and handled 40 research projects and transferred 5 technologies for commercialization. He has guided 21 Ph.D. and 60+ M.Tech. students. Prof. De has been awarded several awards, including Institute Chair Professorship, 2020, Abdul Kalam Fellowship for Innovative Research 2017, Innovation Award from Indian Desalination Association 2016, INAE Chair Professorship 2015, Innovation Award by Ministry of Chemicals and Fertilizers 2015, Lockheed-Martin top 10 innovation 2015, NASI-Reliance Industries Platinum Jubilee Award (2013), INAE Silver Jubilee Award (2012), DAE-SRC Young Investigator Award (2012), Shanti Swarup Bhatnagar Prize in "Engineering Science" category by CSIR, Govt. of India (2011), Herdillia Award (2010), VNMM Award from IIT Roorkee (2009), Young Engineer Award by INAE (2001). He is a Fellow of Indian National Academy of Engineers, New Delhi and The National Academy of Sciences, India, Allahabad. He is the founder of the spin-off company M/s, Technoquipts Separation Pvt. Ltd.

Cost-effective research instrumentation and materials in India



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Brief Bio-Sketch

Dr. Rajendra Joshi, an instrumentation professional and material's physicist, is the Founder & C.E.O. of RI Instruments & Innovation, Uttarakhand, India, and Managing Director of RINZTECH NZ LTD, New Zealand. He had got University Medal in M.Sc. (Physics) 1996 and his professional career was started from National Physical Laboratory, New Delhi in year 1997. He has more than 19 years of Research and industrial experience in India and abroad in the area of Electron microscopy, material science, nano materials and polymer process. He was awarded Best Engineer (Process) in Turin Italy 2007. Till now he has filled 29 patents and published 19 papers in peer reviewed international journals. He has designed and developed several devices. Few of among these devices are like drones which will help in detecting a natural disaster like cloud burst, graphene nano material based alcohol sensor device, universal spectrometer, several high precession polymer testing instruments and cost-effective instruments like USB microscope, solar simulator, Raman spectrometer etc. He is a recipient of prestigious National Innovation Award for the year 2019 by Ministry of Chemicals and Fertilizer, Government of India for innovation of Graphene Oxide/Li based rechargeable batteries. He is also privileged to be in the list of selected Indian Entrepreneurs so far addressed in House of Lords (United Kingdom) during International Business Meet in London in November 2020. He is also a recipient of UFTARA award by Uttarakhand Government.

Photophysical properties of semiconductor and 2D materials based quantum dots



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In the recent past, there has been an increasing interest in understanding the excited state dynamics of quantum dots (QDs) due to their potential role in energy harvesting and biomedical applications. The present talk summarizes the results obtained from our laboratory regarding the excited state dynamics and emission properties of CdSe QDs, Graphene QDs and novel 2D materials based QDs. The excited state dynamics of CdSe quantum dots (CdSe QDs) were monitored using femto second laser flash photolysis system, in the presence and absence of graphene quantum dots (GQDs). The results from the study indicate the evidence of electron transfer from CdTe QDs to GQDs with the hole-trapping process by surface defects. More importantly, the consequences of improved charge transfer have been established through the measurements of enhanced photoconductivity (i.e. from 1.39 $(\pm 0.12) \times 10^{-4}$ S m⁻¹ in the control system to 1.47 $(\pm 0.24) \times 10^{-3}$ S m⁻¹ in the system under investigation). Preparation of quantum dots from novel 2D materials such as Pyrediyne, and coronene-pyrene hybrid 2D material (COPY) will also be described and their bioimaging applications will be presented.

References

- (a) M. A. Mahato, C. Govind, V. Karunakaran, S. Nandy, C. Sudakar and E. Prasad, *J. Phys. Chem. C*, 2019, **123**, 20512; (b) J. S. Arya, P. Prabakaran, E. Prasad and S. Sankararaman, *Adv. Mater. Interface*, 2020, **7**, 1902209; (c) J. S. Arya, M. K. Mahato, S. Sankararaman and E. Prasad, *J. Mater. Chem. C*, 2021 (just accepted).
- 2. A. Corma, H. Garcia and F. X. Llabresi Xamena, Chem. Rev., 2010, 110, 4606.
- 3. D. N. Dybtsev, A. L. Nuzhdin, H. Chung, K. P. Bryliakov, E. P. Talsi, V. P. Fedin and K. Kim, *Angew. Chem. Int. Ed.*, 2006, **45**, 916.

Brief Bio-Sketch

Prof. Edamana Prasad and did his early education at Calicut University, Kerala. He did his Ph.D. in 2000 from NIIST Thiruvananthapuram, Kerala, India. He did his postdoctoral work from (A) Texas Tech University, Texas, USA; (B) University of Bonn, Germany as AvH Fellow, and (C) Lehigh University, Pennsylvania, USA. He was an Assistant Professor at IIT Madras in 2006. He was an Associate Professor in 2012 and became a full Professor on 2018. Prof. Edamana Prasad and his group works in the area of *supramolecular photophysics*. We focus on rational design and preparation of a variety of self-assembled systems, which include small organic molecules (derivatives of poly cyclic hydrocarbons), macromolecules (dendrons, dendrimers, 2D molecular systems etc.) and organic-inorganic hybrid systems (organo-lanthanides, nanoparticles/quantum dots in gel medium etc.). The research interests include: (i) understand the mechanistic aspects of self-assembled systems for materials applications. He has published a total of 90 peer reviewed journal papers. He has guided 19 Ph.D. student and currently he has 13 Ph.D. student under his guidance.

Carbene-catalyzed kinetic resolution of racemic nitroolefins embedded in chromane and tetrahydroquinoline structures



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Benzofused oxygen- and nitrogen-containing heterocycles are the structural basis for a plentiful number of natural products and synthetic analogues with diverse and often show desirable biological/pharmacological properties. Therefore, a number of metal- or metal free asymmetric methods have been developed. In particular, the double domino/cascade process (oxa-Michael/Michael or oxa-Michael/Henry or aldol condensation) is a choice of method to prepare enantioenriched chromane/2*H*-chromene and 1,2,3,4-tetrahydroquinoline/1,2-dihydroquinoline derivatives¹. However, the domino-strategies employed were not always suitable for the construction of the envisaged functionalized heterocycles. Thus, the incessant exploration and the development of an alternate and efficient method are highly desirable in current context. Last few years, the development of an efficient and catalytic kinetic resolution



Scheme 1. Kinetic resolution of C₂-substituted 2*H*-chromene and 1,2-dihydroquinoline.

(KR) of racemates by *N*-heterocyclic carbenes (NHCs) is an attractive area of research². Inspired by the recent development on the NHC-catalyzed generation of the reactive intermediates and their reactions with nitroalkenes for the construction of high synthetic value building blocks³, we herein report *N*-heterocyclic carbene-catalyzed synthesis of dense-functionalized chromane (**3**), tetrahydroquinoline (**4**) including 2-substituted chromene (*R*)-**1** and 1,2-dihydroquinolines (*R*)-**2** through azoliumhomoenolate pathway (Scheme 1)⁴. In this study, the remote stereocenter in C₂-position of racemic nitroolefins embedded heterocycles is resolved, successfully.

References and Notes

- 1. (a) G. Desimoni, G. Faita and P. Quadrelli, *Chem. Rev.*, 2018, **118**, 2080; (b) C. Bhanja, S. Jena, S. Nayak and S. Mohapatra, *Beilstein J. Org. Chem.*, 2012, **8**, 1668.
- 2. Z. Wang, D. Pan, T. Li and Z. Jin, *Chem. Asian J.*, 2018, **13**, 2149.
- 3. B. Maji, Asian J. Org. Chem., 2018, 7, 70.
- 4. A. Bhattacharya, P. M. Shukla, L. Kaushik and B. Maji, Org. Chem. Front., 2019, 6, 3523.
- 5. P. M. Shukla and B. Maji, (manuscript submitted, 2021).

Brief Bio-Sketch

Dr. Biswajit Maji is an Assistant Professor of Department of Chemistry, Indira Gandhi National Tribal University, Amarkantak, Madhya Pradesh, India, Biswajit Maji was born in West Bengal, India. He accomplished both the UG and PG in Chemistry at the Vidyasagar University, Midnapore, West Bengal. After that he joined in the research group of Prof. SaumenHajra at the Indian Institute of Technology, Kharagpur, India, and received Ph.D. degree in 2010. Next, he moved as a postdoctoral research fellow to Nanyang Technological University (NTU), Singapore. In NTU, he spent more than two and half years working on nucleophilic organocatalysis project. In October, 2012, he returned as an Assistant Professor, Department of Chemistry, Indira Gandhi National Tribal University, Amarkantak, Madhya Pradesh (A Central University). In 2013, he has been awarded DST-INSPIRE Faculty to start research career. His research interests include the asymmetric synthesis and catalysis and very recently focusing on inert C-F bond activation or functionalization at C₃-center of oxindole to access enantioenriched fluorinated oxindole.

Multifunctional nanocomposites





With the required miniaturization, the materials combining different functionalities have become interesting. In this topic, a variety of advanced polymer nanocomposites will be introduced. Methodologies to prepare nanocomposites and their effects on the produced nanocomposites will be introduced. Unique properties including mechanical, electrical, magnetoresistance etc. and the applications for environmental remediation, energy storage/ saving and electronic devices (Sensors and Electrochromic Display Windows) will be presented.

Brief Bio-Sketch

Dr. Guo, currently an Associate Professor in Chemical & Biomolecular Engineering Department of at the University of Tennessee (UT), obtained his Bachelor degree from Shan-dong University of Science and Technology (1996), Master degree from Beijing University of Chemical Technology (1999), and Ph.D. degree from Louisiana State University (2005). All the degrees were from Chemical Engineering. Before joining UT, Dr. Guo was working in Lamar University from 2008-2014 as Assistant/ Associate Professor in Dan F. Smith Department of Chemical Engineering. Meanwhile, Dr. Guo had received a three-year (2005-2008) postdoctoral training in the Mechanical and Aerospace Engineering Department at the University of California Los Angeles. Dr. Guo directs the Integrated Composites Laboratory (ICL) and has authored/coauthored more than 800 peer-reviewed journal papers and five issued patents. The scientific results have been reported by major media including Nanotechweb by the Institute of Physics (IOP), Plastics Engineering Magazine by the Society of Plastics Engineering (SPE), MaterialsViews by Wiley, National Science Foundation (NSF), etc. Dr. Guo has received Honorary Nomination Award of 2007 for UCLA-Chancellor Research, University Merit Award of 2012 for teaching, and University Scholar Award of 2013 for research at Lamar University. Dr. Guo had served as Chair for the Composites Division of AIChE (2011-2012). Dr. Guo's current research team focuses on multifunctional light-weight nanocomposites, especially with polymer and carbon as the hosting matrix to solve the energy and sustainability issues. The research activities have been supported by NSF, American Chemical Society (ACS) Petroleum Research Fund (PRF), and several global industrial companies. For more information, please visit http://composites.utk.edu.

Lessons learned from functional modelling of galactose oxidase enzyme: Design and synthesis of new catalysts for organic synthesis

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Galactose oxidase enzyme (GOE) is an important fungal enzyme which is responsible for catalytic conversion of D-galactose to D-galacto-hexodialdose. Structural and functional modelling of GOE received considerable current attention for the synthesis of carbonyl compounds under mild conditions¹. Hydrogen atom transfer (HAT) mechanism and role of phenoxyl radical are important aspects of the catalytic cycle². Role of non-innocent ligands in metal complexes were also reported for the synthesis of carbonyl compounds³. In situ generated carbonyl compounds were utilized for guinolone synthesis, N-alkylation and α alkylation reactions⁴.



References

- 1. (a) K. Ghosh, P. Kumar, V. Mohan, U. P. Singh, S. Kasiri and S. S. Manal, Inorg. Chem., 2012, 51, 3343; (b) K. Ghosh, P. Kumar, N. Tyagi and U. P. Singh, Inorg. Chem., 2010, 49, 7614.
- 2. L. Que (Jr.) and W. B. Tolman, Nature, 2008, 455, 333.
- 3. (a) D. Sengupta, R. Bhattacharjee, R. Pramanick, S. P. Rath, N. S. Chowdhury, A. Datta and S. Goswami, Inorg. Chem., 2016, 55, 9602; (b) R. Pramanick, R. Bhattacharjee, D. Sengupta, A. Datta and S. Goswami, Inorg. Chem., 2018, 57, 6816.
- 4. (a) A. Maji, A. Singh, N. Singh and K. Ghosh, *ChemCatChem.*, 2020, **12**, 3108; (b) A. Singh, A. Maji, M. Joshi, A. R. Choudhury and K. Ghosh, *Dalton Trans.*, 2021, 50, 8567.

Brief Bio-Sketch

Dr. Kaushik Ghosh is a Professor of Department of Chemistry and (Joint Faculty) Department of Biosciences and Bioengineering, Indian Institute of Technology Roorkee, Roorkee 247 667, Uttarakhand, India. He did his Ph.D. from Indian Association for the Cultivation of Science (IACS), Calcutta, India on 2001 under the supervision of Prof. Animesh Chakravorty. He did his M.Sc. from Indian Institute of Technology (IIT), Kanpur, India on 1996. He did his B.Sc. from University of Kalyani, West Bengal, India on 1993 and he achieved Gold Medal during his B.Sc degree. He did his postdoctoral work at Magnetic Resonance Centre, University of Florence, Italy with Professor Ivano Bertini in NMR structural biology from 2000 to 2002. He did his second postdoctoral work at Department of Chemistry and Biochemistry, University of California at Santa Cruz (USA) with Professor Pradip K. Mascharak and Professor Ted Holman from 2002 to 2005. He was an Assistant Professor and Associate Professor at IIT Roorkee from 2006 to 2012 and 2012 to 2018 respectively. His research interests are - Coordination chemistry, Metal complexes in nitric oxide (NO) research, Organometallic chemistry and catalysis and Protein misfolding and role of metal ions. He has got several prestigious awards. He is the Recipient of Certificate of Merit from University of Kalyani: Topper (First Class First, Gold Medallist) in B.Sc. (Honours in Chemistry) in the year 1993. He was Awarded DST-SERC Fast Track Scheme for Young Scientists (FAST) on 2007. He was a Visiting faculty at LCC CNRS Toulouse France as ICMR International fellow from 2012 to 2013.

Chemistry of Oil Refining

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With almost a year in the era of BS VI diesel and gasoline specifications in India, it is worthwhile to take a look at the technologies that were helpful in achieving the almost impossible target of meeting BS VI specifications for gasoline diesel within a very short span of time. It is noteworthy to understand that in spite of arrival of newer challenges to so-called conventional liquid hydrocarbon fuels in the energy sector, the hydrocarbon fuels like diesel and gasoline will be mainstay with major chunk coming from the fossil fuels. It was a formidable task for refineries to meet the advanced BS VI specifications. The journey has been eloquently explained in the presentation by revisiting the basic chemistry, basic chemical engineering fundamentals for each and every technology candidate and their role in achieving the specification targets. It has been also highlighted that all those latest developments in each technology had to be done by analyzing the existing refinery infrastructure of each technology unit in the refinery. Each property of both the fuels has been discussed and how they affected the final selection of technological unit, simultaneously analyzing the existing status of each technology unit by revisiting the all the parameters separately has also been discussed. The catalyst function, design, and development for each technology have been visited. The reactor design and unit configuration changes according to the requirement have also been explained. Finally, the impact on the refinery in terms of developments and challenges in associated units, like hydrogen generation unit, sulfur recovery units, etc., have also been touched upon highlighting the possible opportunities. The discussion further dwells on the bottom of the barrel upgradation technologies such as delayed coking and resid hydrocracking in the new light of BS VI specifications. The delayed coker can also be source of novel value added products like anode grade coke in addition to its conventional role as fuel producing technology. In addition to the technologies available from other licensors worldwide, the discussion enlists the technology basket on the offer from Indian Oil. All these developments and possible shift in product slate in light of energy efficiency and environmental regulations coupled with the internet of things, the future refinery may look radically different than what it was few years back and may be constituting the guite a different energy sources like renewables (fuel and electricity), hydrogen, etc. and some of the upcoming areas of research have been touched upon. Accordingly, the refineries of the future would be more R&D driven.

Brief Bio-Sketch

Dr. S. S. V. Ramakumar is Director (Research & Development) on the Board of Indian Oil Corporation Ltd. (Indian Oil), a Fortune 500 company.

Dr. Ramakumar has more than three decades of uninterrupted R&D experience in downstream hydrocarbon sector, notably in the areas of lubricant technology, refinery process research streams, including catalyst development. He is instrumental in developing India's home-grown, OEM-approved marine lubricant technology, which catapulted Indian Oil's SERVO lubes into the select league of five MNC oil companies. He spearheaded the complete indigenization of Indian Oil's flagship resid up-gradation technology - INDMAX by way of developing in-house catalyst for the process. Under his able guidance, IndianOil has developed bouquet of technologies for producing BS VI quality fuels in the refineries. He spearheaded the fastest ever development and commercial deployment of Indane Nanocut high-therm metal-cutting gas. On-purpose technologies like Octamax for octane enhancement of MS pool, differentiated LPG for domestic applications. He is leading a team of scientist to develop cutting edge solutions in energy storage (batteries), hydrogen and fuel cells and solar energy. Dr. Ramakumar is currently steering the setting up of Centre of Excellences in Alternative Energy, nanotechnology and Synthetic Biotechnology and Corrosion Research at the 2nd R&D campus of Indian Oil.

Dr. Ramakumar has to his credit over 150 research publications in peer reviewed national/ international journals and 142 granted patents besides winning several prestigious awards for presenting the best research papers in international conferences. Apart from serving on Indian Oil Board, Dr. Ramakumar is also a Board member of Lanzatech, USA, Board member of Central Pollution Control Board (CPCB) and is also on the Board of Oil Industry Development Board (OIDB) besides presiding the activities of industry bodies like Society for Petroleum Laboratories and India Energy Forum. He is also currently a member of Executive Council of PCRA, member of National APEX Council of Prime Minister Research Fellowship Scheme for doctoral programme, member of Nano Applications and Technology Advisory Group (NATAG), member of Research Advisory Board (RAB) of ICAT, under Scientific and Research Organisation (SIRO), Convener of Methanol utilization task force constituted by NITI Aayog, Adjunct Professor at Institute of Chemical Energy, Mumbai & Bhubaneswar Campuses, Professor of Practice and Senate Member of IIT-Delhi, Chairman Bio-ATF Task Force, Chairmanm, SAE India Think Tank and Chairman, Green Hydrogen and Sourcing of Hydrogen expert committees setup by MoPNG and MNRE respectively. Dr. Ramakumar also heads the DBT-IOC Bio-Energy Research Centre and is on the Governing Council of International Centre for Genetic Engineering and Bio-technology (ICGEB), Governing Council member for Centre of Excellence in Advanced Biofuels and Biocommodities and Governing Council member of Centre of Excellence in Oil, Gas and Energy, IIT Mumbai. Several national scientific societies like International Council of Internal Combustion Engines - India Chapter (CIMAC INDIA), Indian Society of Fuels and Lubricants (ISFL), Tribology Society of India (TSI) are currently being presided over by Dr. Ramakumar.

Dr. Ramakumar who recently has been conferred with Fellowship of National Academy of Engineering has received many awards, including NPMP, FIPI, NRDC, AIIMA Innovation, Bangalore Nano, and WPC Excellence Award for product and process technologies he developed.

Competitive advantage of FSRU (Floating Storage Regasification Unit) over onshore LNG terminal

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In recent years the gas transportations in the form of liquefied natural gas (LNG) have increased due to the transcontinental requirements. However, the construction of onshore LNG terminals may often face several issues including the local resistances due to fears of explosions. Several gas importers may then think alternatively to join the global LNG market through the addition of floating storage regasification unit (FSRU) instead of conventional onshore LNG terminals. Both onshore LNG terminals and FSRUs have distinct benefits and drawbacks. The FSRUs often chartered from third parties are typically less capital-intensive than onshore developments and can often be completed via faster permitting processes. The capital expenditures for FSRUs may be lower than onshore, due to potential construction cost efficiencies through repeatability gains where there is a generic design concept, with minor adaptations for each specific project and so on. FSRU costs can also be betterly controlled with construction/assembly activities that are organized through designated shipyards and supply chains using established labour and materials resources. There is no need to purchase or lease waterfront land for creating onshore facilities. FSRUs also can provide flexibility to terminal operators to release the vessel if regasification capacity is no longer required. The study concludes that FSRUs are better alternatives in comparison to onshore LNG terminals.

Brief Bio-Sketch

Ashanendu Mandal is graduated as B.Sc. (Chemistry) and B.Tech. (Chemical Engineering) from University of Calcutta and post-graduated as M.Tech. (Chemical Engineering) from IIT, Kharagpur. He has acquired MBA degree in Finance from IGNOU, New Delhi and also Advanced Management Program from IIM, Calcutta. Mr Mandal has worked in ONGC for more than 34 years. His experience includes commissioning, modifications, safety, operations, artificial lifts, pressure maintenance, EOR and planning in offshore and onshore oilfields. He has also vast experience in marketing of upstream and downstream petroleum products. Mr. Mandal has attended several upstream training programs in USA, Canada, Singapore, Netherlands, Norway, France and Belgium. He has participated as

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invited speaker in many international conferences held in Abu Dhabi, Amsterdam, Bahrain, Bangkok, Barcelona, Cape Town, Dubai, Jakarta, Kuala Lumpur, London, Paris, Perth, Shanghai, Shenzhen, Singapore, Terengganu and Yangon. Mr. Mandal has published technical papers in Chemical Weekly and is the lifetime professional member of Indian Chemical Society and Indian Science Congress. He received the Best Researcher Award by VD Good International Professional Association in the year 2020.

Polycyclic aromatic hydrocarbon derivatives: A versatile donor and acceptor molecules for organic electronic materials





Polycyclic aromatic hydrocarbons (PAHs) are rich source of π -electrons due to inherent aromatic character of the compounds. Because of large π -electron cloud and sp² planar geometry of the molecules force them to self-assemble to form disc shaped three dimensional structure. The disc shaped self-assembled structure favours the electron-hole transport through the core π -electron cloud. However, the solubility and electron-hole transport is much limited due to larger structure and electronically neutral nature of the PAHs. The poorer solubility of the PAHs reduce the solution processibility for the electronic applications. Our objective is to introduce the heteroatom such as N and S in the PAHs and increase the solubility of PAHs such as hexa-*peri*-hexabenzocoronene (HCBs) and perylene diimide molecules (PDIs) to improve the solution processable electronic properties of these molecules. The optoelectronic properties of these molecules especially PDIs studied using UV-Vis absorption and fluorescence, life time measurements and TOF-electron transport properties. PDIs substituted with electron donating substituents showed good electron transport properties in its spin coated amorphous thin film state.



Figure. (a) Perylene diimide molecules and (b) TOF-electron mobility measurements.

Brief Bio-Sketch

Dr. V. Sivamurugan is graduated in Chemistry from University of Madras. In the year 2005, he received Doctorate in Organic Chemistry from Anna University, Chennai in the field of heterocyclic compounds synthesis. Then, he joined as a Research Fellow in National University of Singapore in September 2005. He actively involved in the synthesis of perylene diimide based electron transport molecules until July 2009. From August 2009 to Januaray 2014, he served as a Senior Research Scientist in DyStar Singapore Pte Ltd and contributed to the design of novel eco-friendly textile dyes. Since January 2014, he is serving as Assistant Professor in the Department of Chemistry, Pachaiyappa's College, Chennai. He is currently working in organic electronic materials, environmental catalysis and structural elucidation of natural products. He received prestigious Fellow of Indian Chemical Society (FICS) in October 2017. He has published more than 60 international research articles in the reputed journals in the field of catalysis, molecular electronics and marine natural products extraction. He filed more than 22 international patents from the textile dyes design and synthesis. He has hindex 14 and i10-index 16 with more than 1250 citations. One of his collaborative research works on bio-emulsifier and anti-cancer drug structure elucidation published in *Scientific Reports* in the year 2018 and 2021.

Inorganic Chemistry Section

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Inorganic Chemistry Lecture-1

Synthesis, characterization of mononuclear copper(II) complexes as a potential nucleic acid binding agent

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Azo linked salicyldehyde and a new 2-hydroxy acetophenone based ligands (HL¹ and HL²) with their copper(II) complexes $[Cu(L^1)_2]$ (1) and $[Cu(L^2)_2]$ (2) were synthesized and characterized by spectroscopic methods such as ¹H, ¹³C NMR, UV-Vis spectroscopy and elemental analyses. Calculation based on Density Functional Theory (DFT), have been performed to obtain optimized structures. Binding studies of these copper(II) complexes with calf thymus DNA (ct-DNA) and torula yeast RNA (t-RNA) were analyzed by absorption spectra, emission spectra and Viscosity studies and Molecular Docking techniques. The absorption spectral study indicated that the copper(II) complexes of 1 and 2 had intrinsic binding constants with DNA or RNA in the range of $7.6\pm0.2\times10^3$ M⁻¹ or $6.5\pm0.3\times10^3$ M⁻¹ and $5.7\pm0.4\times10^4$ M⁻¹ or $1.8\pm0.5\times10^3$ M⁻¹ respectively. The synthesized compounds and nucleic acids were simulated by molecular docking to explore more details mode of interaction of the complexes and their orientations in the active site of the receptor.

Reference

 Synthesis, characterization and nucleic acid binding studies of mononuclear copper(II) complexes derived from azo containing *O*, *O* donor ligands, *Nucleosides, Nucleotides and Nucleic Acids*, 20018, 37(10), 563.

Inorganic Chemistry Lecture-2

Cyclometallated iridium and platinum complexes containing ppy type ligands

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Iridium and platinum complexes have drawn attraction due to potential application in various fields. Cyclometallated iridium and platinum complexes 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) and platinum(II) complexes have been commonly used as light emitting material in common Organic light-emitting diodes (OLEDs) due to their high quantum efficiency¹. They show various range of tunable light emission by different type of attached ligands. The strong spin-orbit coupling induced fast intersystem crossing (ISC) causes iridium complex as luminescence materials². Phosphorescence emission is caused by mixed excited triplet states i.e. LC and MLCT. Now 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.

References

- 1. C. Adachi, M. A. Baldo, S. R. Forrest and M. E. Thompson, Appl. Phys. Lett., 2000, 77, 6904.
- 2. S. Tokito, Y. Sakamoto, T. Suzuki and Y. Taga, Appl. Phys. Lett., 2001, 79, 156.

Inorganic Chemistry Lecture-3

Nickel based chalcogenide electrodes with porous nano architecture as a battery-type cathode for pouch-type hybrid supercapacitor and upcycle of the generated E-waste into antibacterial material

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Nickel based chalcogenide nanostructures were supported on highly conductive nickel foam. They were synthesized using facile chemical bath deposition technique. The densely grown nanostructure, with its large number of electroactive sites, facilitated rapid diffusion and charge transport. The Ni based chalcogenide electrode, exhibited a superior specific capacitance value of 2704 F g⁻¹ at a current density value of 4 mV s⁻¹ in a 1 *M* aqueous KOH electrolyte. Furthermore, a high-energy-density pouch-type hybrid supercapacitor (HSC) device was fabricated using the proposed battery-type NiSe-Se@NiO@Ni foam as the positive electrode, activated carbon on Ni foam as the negative electrode, and a filter paper separator soaked in a 1 *M*KOH electrolyte solution. The HSC delivered a specific capacitance of 91.68 F g⁻¹ at a current density of 6 mA cm⁻² with an energy density of 0.52 mWh/cm² at a power density of 22.9 mW/cm² for an extended operating voltage window of 1.6 V. In addition, the HSC exhibited excellent cycling stability with a capacitance retention of 93.87% after 5000



cycles, highlighting its excellent potential for use in the hands-on applications. The real-life practicality of the HSC was tested by using it to power a red light-emitting diode, a toy motor fan and a PC cooler fan. Further, the used electrodes (E-waste) were upcycled and converted into antibacterial material. The upcycled electrodes were tested against *E. coli* bacteria. The recycled electrodes showed excellent antibacterial property.
New water soluble bridged dicopper(II) assemblies for the exploration of amino-sugar/metal ion interactions

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Employing a carboxylate-based multidentate ligand N, N-bis[2-carboxybenzomethyl]-N, Nbis[2-pyridylmethyl]-1,3-diaminopropan-2-ol (H₃cpdp), new water-soluble dimetallic copper(II) complexes, $[Cu(H_2O)_5][Cu_2(cpdp)(\mu-O_2As(CH_2)_2)]_2Br_2 \cdot 13.83H_2O \cdot 0.67CH_3OH$ (1) and $[Cu_2(Hcpdp)(\mu - SO_4)] \cdot 5H_2O(2)$ and $[Cu_2(cpdp)(\mu - pz)] \cdot 16H_2O(3)$, where $(CH_3)_2AsO_2^- =$ cacodylate; SO_4^{2-} = sulfate; pz⁻ = pyrazolate have been prepared and characterized for the investigation of coordination/binding aspects with biologically relevant amino-monosaccharide, D-glucosamine. Diverse analytical methods, such as elemental analysis, thermogravimetry, FTIR, UV-Vis and mass spectrometry, magnetic measurements and X-ray crystallography, have been utilized to characterize these complexes. Temperature dependant (2–300 K) magnetic susceptibility measurements reveal the presence of antiferromagnetic interactions between the copper centers in 1 and 2. Thermogravimetric analysis of 1-3 shows that they are stable on average up to ~214°C. UV-Vis spectroscopic technique has been successfully applied to study the 1:1 interactions of the complexes with D-glucosamine in solution. The binding constant values evaluated from the experimentally obtained UV-Vis titration data are 2.019×10^3 M⁻¹, 1.519×10^3 M⁻¹ and 2.457×10^3 M⁻¹ that correspond to the amino sugarbound complexes 1/D-glucosamine, 2/D-glucosamine and 3/D-glucosamine, respectively. Fukui functions at the metal sites, including HOMOs and LUMOs in 1-3 have been calculated by DFT method to indicate the possible metal centers involved in the binding process with Dglucosamine.

References

- 1. A. Patra, T. K. Sen, A. Ghorai, G. T. Musie, S. K. Mandal, U. Ghosh and M. Bera, *Inorg. Chem.*, 2013, **52**, 2880.
- 2. A. Patra and M. Bera, *Carbohydr. Res.*, 2014, **384**, 87.
- 3. G. C. Giri, S. Haldar, G. Vijaykumar and M. Bera, *ChemistrySelect*, 2017, 2, 2847.

Exploration of water quality from the effluents of Sirgitti Industrial Region in Bilaspur (Chhattisgarh)

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Analytical studies of some selected physicochemical parameters were done on the surface water bodies of Sirgitti Industrial Region, Bilaspur, Chhattisgarh. Water samples were collected from four different selected spots in June'2020 of pre-monsoon season, were explored for physicochemical and heavy metal like Fe, Zn, Mn and Al by the standard method as per IS procedure. More than 70% of these parameters were exceeding the permissible limit of BIS: 10500 and WHO standard of drinking water. The higher values of these parameters are of great concern to public health. Removal of water pollutants has been done by preparing bioadsorbents from local plant origin. Adsorption capacity of different adsorbents has been established and compared for the removal of various pollutants. The changes in pH, colour, COD, TS, TDS, TSS, TA, TH, Chloride, fluoride, sulphate, nitrate, phosphate, Ca, Mg, Na, K and heavy metals e.g. Cu, Zn, Fe, Al etc. have been observed.

Surface functionalized silver nanoparticles as colorimetric probe for selective determination of L-cysteine in milk samples

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A simple and sensitive colorimetric method has been established for selective detection of L-cysteine (Cys) using ionic liquid functionalized silver nanoparticles (ILs-AgNPs). The sensing mechanism is dependent on the change in color of NPs and shifting of absorption band was observed from 395 nm to 560 nm in the visible region. The synthesized ILs-AgNPs was characterized in the absence and presence of Cys using UV-Vis, Fourier transformsinfrared (FT-IR) spectroscopy, transmission electron microscope (TEM) and dynamic light scattering (DLS). The analytical performance of the proposed sensing approach has also been investigated at the linear range of 10–100 ng mL⁻¹ and detection limit was observed to be 4.72 ng mL⁻¹. Furthermore, binding mechanism has also been studied using UV-Vis technique. The proposed strategy possesses advantages of simplicity and selectivity and hence it will be applied for analysis of Cys in milk samples.

Electrochemical ammonia synthesis by nitrate reduction using iron phthalocyanine catalyst

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Electrocatalytic conversion of nitrates a typical notorious water pollutant into value added chemicals is an effective strategy to balance the nitrogen cycle but to optimize the product selectivity remains a challenge. The effective conversion of nitrates to ammonia is a greener route and can be a probable alternate for the Haber-Bosch process. As there are many pathways of nitrate reduction, selectivity is very important. The site-specific selective pathway leading to ammonia formation is lacking due to the lack of effective electrocatalyst.

In this report, we present iron phthalocyanine as a potential electrocatalyst capable of showing selective reduction of nitrate to specifically ammonia with yield rate of NH₃ and Faradic efficiency of 166 μ g h⁻¹ mg⁻¹ cat and 91% respectively at –0.01 V vs RHE using 0.1 MK₂SO₄ containing 200 ppm KNO₃ as an electrolyte.

Recent advances in the synthesis of 3d-4f heterometallic complexes using compartmental ligand approach and their applications

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In recent decades 3d-4f heterometallic discrete complexes have growing special attraction in the field of molecular magnetic materials with potential applications in the information storage device, guantum computer, spintronics, and magnetocaloric materials. The significant magnetic anisotropy of Ln(III) ions like Tb(III), Dy(III), Ho(III), Gd(III), Yb(III) and Er(III) ions allowed the synthesized complexes as captivating candidates to construct molecular nanomagnets. Compartmental ligands like phenol-based Schiff bases are useful candidates in the construction of 3d-4f heterometallic multinuclear complexes as there are different pockets are available for different types of metals according to the hard and soft acids and bases (HSAB) principle. 4f ions like Tb(III), Dy(III), Ho(III) and Er(III) prefer hard pockets and preferentially interact with the oxygen-rich parts of ligands, while 3d ions like Cu(II), Ni(II), Fe(II), Co(II) and Mn(III) prefer soft donor atom-like nitrogen atoms for binding. Although the study of 3d-4f heterometallic complexes is a well-established field as many databases related to the structural topology and nanomagnet materials are available in the literature, still, we believe that a lot of effort remains to be carried out on the development and understanding of the complicated magnetic exchange interactions between the 3d and 4f spin carriers and subsequent theoretical computational simulation of the observed magnetic behaviours. Here we review the synthetic approaches, structural topology, and magnetic properties of 3d-4f heterometallic discrete complexes.

References

- 1. Avik Bhanja, Michael Schulze, Radovan Herchel, Eufemio Moreno-Pineda, Wolfgang Wernsdorfer and Debashis Ray, *Inorg. Chem.*, 2020.
- 2. Dipmalya Basak, Jan van Leusen, Tulika Gupta, Paul Kogerler, Valerio Bertolasi and Debashis Ray, *Inorg. Chem.*, 2020.
- 3. Dipmalya Basak, Jan van Leusen, Tulika Gupta, Paul Kögerler, Debashis Ray, *Dalton Transaction*, 2020.
- 4. Avik Bhanja, Radovan Herchel, Zdenek Travnícek and Debashis Ray, Inorg. Chem., 2019.
- 5. Ke Liua, Wei Shia and Peng Cheng, Coord. Chem. Rev., 2015, 289-29, 74-122.

Studies of Ni(II) complex – synthesis, spectral studies and antimicrobial activities

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A new series of transition metal complex of Ni(II) was synthesized from the Schiff base ligand derived from salicyaldehyde and 2-aminothiophenol. Ligand and its metal complex have been evaluated by analytical data, conductivity measurement, magnetic moment, IR, electronic spectra, XRD and thermal studies. Analytical data confirmed 1:2 (metal:ligand) stoichiometry and the spectral data suggest that Ni(II) complex has octahedral geometry. Antibacterial, antifungal and antioxidant activities of the ligand and its metal complex were performed *in vitro* against *E. coli, S. typhi, S. aureus, B. subtilis* and against various fungi like *P. chrysogenum, A. niger, F. moniliformae* and *A. Flavus.* The complex has been found to be more activity as compared to the ligand.

F---F Interaction in superstructure of fluorinated triazolylpyridyl Mn(II) coordination compound and Schottky diode effect

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Pyridyl appended triazoles are planar aromatic surface favoring π - π stacking molecules and have recently been used to synthesise metal complexes of varying three-dimensional structures. 1,2,4-Triazole designs range of coordination polymers consisting 1D, 2D and 3D coordination polymers. Such architectures exhibit potential application in the areas of catalysis, absorption, magnetism, molecular recognition, optic sensors, energetic materials, electrical conductivity, medicine, gas storage, and nonlinear optical (NLO) activity. Fluorinated organic coordinating ligands have several advantages for their pharmaceutical ability and utilisation as agrochemicals. In this report, the crystal structure of the fluorinated compound is presented, namely, [Mn(H₂O)₂(PyTrCF₃)₂], (PyTrCF₃ = 2-(5-trifluoromethyl-4h-[1,2,4]triazol-3-yl)pyridine). Hydrogen bonding, π π conjugation, F----F bonding are an excellent noncovalent interaction that forms supramolecular architectures. In crystal the F.....F (2.98 Å and 3.36 Å) are found to be comparable with the sum of the corresponding van der Waals radii (2.94 Å) and the C-F....F (132° and 120° respectively) contacts are also deviated from linearity. In the dark condition, the conductivity of the device is 1.76×10^{-5} Sm⁻¹ and after



Fig. 1. (a) Coordination sphere around the Mn(ι) ion with π·····π aggregation, H-bonding interactions in 1.
(b) F·····F interaction in crystal system.

irradiation of light, the conductivity is 4.47×10^{-4} Sm⁻¹. The photosensitivity of the device is found to be 23.52 at 1000 Wm⁻² illumination.



Fig. 2. (a) Current-Voltage (I-V) characteristic curve under the dark and light condition and (b) I (log scale) vs V plot for complex.

Photochromic, photovoltaic and photophysical activities of 2-(coumarinyl-6-azo)-4-substituted imidazole or 1-alkyl-2-(coumarinyl-6azo)-4-substituted imidazole ligands and its osmium and iridium complexes

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The chemistry of 2-(coumarinyl-6-azo)-4-substituted imidazole or 1-alkyl-2-(coumarinyl-6-azo)-4-substituted imidazole ligands as well as its metal complexes are fascinating. All the ligands are fluorescent and also exhibit photochromic behaviour. The quantum yield of E-Z isomerization is sensitive to substitution on imidazole ring. The iridium and osmium carbonyl complexes of the ligands shows very high fluorescence quantum yield. The ligand and the osmium carbonyl complexes are also display photovoltaic effect and the power conversion efficiency of the osmium complexes are higher than that of the ligands.



Figure. Diagram of 1-alkyl-2-(coumarinyl-6-azo)-4-substituted imidazole ligand (A), X-ray crystallographic structures of iridium (B) and osmium complexes (C) of the ligand.

Synthesis of boron-nitrogen co-doped graphene quantum dots as rapid fluorescence probe for detection of paraoxon

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A simple one-pot synthesis procedure of boron-nitrogen co-doped graphene quantum dots (B,N-GQDs) as fluorescent probe for rapid detection of paraoxon has been explored. The GQDs has been synthesized using citric acid as carbon precursor, boric acid as boron and urea for nitrogen source. The synthesized B,N-GQDs have been characterized by fluorescence, UV-Visible spectroscopy, Fourier transform infrared (FT-IR) and dynamic light scattering(DLS). The method has been applied for detection of paraoxon which is based on the fluorescence quenching of B,N-GQDs. We have also studied the selectivity of B,N-GQDs to paraoxon over other interfering radical have been studied. The analytical performance of this study has been carried in the concentration range of paraoxon from 0.1 to 1000 μ M and a lower limit of detection has been obtained.

Ruthenium(II) complexes of an ambidentate and flexidentate *o*-phenylenediamine-thiophene derivative: Dehydrogenation, *cis-trans* isomerism, C-H activation, imine to imidic acid conversion, dinitro and [RuNO]⁷ complexes

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The versatile redox activities of $(R_1)CH=N-C_6H_4-NH-C(H)(Ph)(R_2)$ (L_1H) , an ophenylenediamine derivative where R_1 = thiophene and R_2 = pyridine functions, that exhibits flexidenticity and ambidenticity towards ruthenium(II) ion and undergoes oxidative dehydrogenation (OD) of the amine function, thiophene metalation via C-H activation, imine \rightarrow imidic acid conversion and affords dinitro and [RuNO]⁷ complexes are reported. Reaction of L_1H with $[Ru^{II}(PPh_3)_3Cl_2]$ (Ru^P) in boiling toluene in air promotes OD reaction affording cis-[Ru^{II}(L₂^{NNN 0})(PPh₃)Cl₂] (cis-1), where L₁H has been modified to (R₁)CH=N-C₆H₄-N=C(Ph)(R_2), a neutral [NNN] donor *o*-phenylenediimine derivative ($L_2^{NNN^0}$). The same reaction at room temparature furnishes the *trans* analogue, *trans*-[Ru^{II}($L_2^{NNN^0}$)(PPh₃)Cl₂] (trans-1). Conversion of trans-1 \rightarrow cis-1 has been achieved in boiling xylene. Reaction of *cis*-1 with I_2 and PPh₃ in toluene produces [Ru^{II}(L₂^{NNNS 0})(PPh₃)CI]I₃ ($\mathbf{3}^+I_3^-$), where L₁H has been modified to $(R_1)CH=N-C_6H_4-N=C(Ph)(R_2)$, a neutral tetradentate [NNNS] donor ligand $(L_2^{NNNS 0})$, where the coordination of thiophene to ruthenium(II) ion has been achieved. Reaction of L₁H and Ru^P in boiling ethanol promotes a C-H activation reaction generating a thiophene metallated complex, trans-[Ru^{II}(L_2^{NNNC})(PPh₃)₂]⁺ (trans-2⁺), where, L_1 H has been modified to a tetradentate [NNNC] donor ligand (L_2^{NNNC}). The same reaction in presence of excess NaNO₂ promotes OD and chloride substitution reactions affording a *cis*-dinitro complex, cis-[Ru^{II}(L₂^{NNN 0})(PPh₃)(NO₂)₂] (cis-4), while the same reaction in presence of HCIO₄ promotes OD and the oxidation of the imine to imidic acid reactions producing a [RuNO]⁷ complex of the type $[Ru^{II}(L_{OH}^{NNN 0})(PPh_3)(NO)CI]^+$ (5⁺), where L₁H has been modified to $(R_1)(OH)C=N-C_6H_4-N=C(Ph)(R_2)$, o-phenylene-imine-imidic acid derivative $(L_{OH}^{NNN 0})$. The molecular structures of all the complexes were confirmed by single crystal X-ray crystallography and the electronic structure of 5⁺ ion was investigated by EPR spectroscopy and DFT calculations.

Organic Chemistry Section

[1 - 14]

Physicochemical evaluation of roots of *Careya arborea* Roxb.

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Careya arborea Roxb. root extracts and its solvent fractionates were subjected to physicochemical and preliminary phytochemical screening using standard methods. The present study deals with physicochemical evaluation of *Careya arborea* Roxb. roots including determination of loss on drying, ash values and extractive values, organoleptic properties and fluorescence analysis. The qualitative chemical examinations revealed the presence of various phytochemical such as alkaloid, terpenoids, saponins, flavonoids, steroids, phenolic compounds, carbohydrates and glycosides in the root extract of the *Careya arborea* Roxb. plant. The presence of several bioactive components endorses the application of *Careya arborea* Roxb. for various diseases by traditional herbal healers. The study revealed specific identities for the particular crude drug which will be suitable in identification and control to depreciate of the raw drug.

Development of industrially viable polymers via utilization of carbon dioxide

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The present study outlines the methodology for the synthesis of a novel family of catalysts that enable the utilization of CO_2 as a C_1 -feedstock. The aim is to thereby improve properties of industrially important polymers such as polyurethanes that contain CO_2 captured from the atmosphere to the extent of at least 10 percent by weight of the product and to establish a deep understanding of structure-property relationships for the catalyst and the final polymers such as polyurethanes (PU).

References

- 1. https://ourworldindata.org/grapher/temperature-anomaly?time=1989..latest(Weblink).
- 2. https://www.climate.gov/news-features/understanding-climate/climate-change-atmospheric-carbondioxide (Weblink).
- M. E. Boot-Handford, J. C. Abanades, E. J. Anthony, M. J. Blunt, S. Brandani, N. Mac Dowell, J. R. Fern andez, M.-C. Ferrari, R. Gross and J. P. Hallett, *Energy Environ. Sci.*, 2014, 7(1), 130e189. https://doi.org/10.1039/C3EE42350F.
- 4. Prakash Alagi, Ravindra Ghorpade, Ye Jin Choi, Umakant Patil, Il Kim,§ Joon Hyun Baik,%" and Sung Chul Hong; *ACS Sustainable Chem. Eng.*, 2017, **5**, 3871. doi: 10.1021/ acssuschemeng.6b03046.
- 5. M. A. Subhani, C. Gürtler, W. Leitner and T. E. Müller, Eur. J. Inorg. Chem., 2016, 1944.

Enzyme catalyzed thioamidation of peptide backbones

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Thioamide as a post-translational modification (PTM) is extremely rare in biological chemistry. Apart from a few peptidic ribosomal and non-ribosomal natural products and some nucleosides, thioamide PTM has been reported in two protein assemblies: the *Escherichia coli*ribosome and methyl coenzyme M reductase (MCR) from methane-metabolizing archaea¹. Compared to an amide, thioamides alter the physical and chemical properties of peptide backbones, including the conformation dynamics, proteolytic stability, hydrogen-bonding capabilities, and possibly reactivity of a protein or peptide compound when installed¹.

MCR is an essential enzyme found strictly in methanogenic and methanotrophic archaea. MCR catalyzes a reversible reaction involved in the production and consumption of the potent greenhouse gas, methane. The α subunit of this enzyme (MCR α) contains several unusual PTMs, including a thioglycine¹. In this talk, *in vitro* reconstitution of the regiospecific thioamide installation on the MCR α peptide backbone (thioglycine) using recombinant YcaO/TfuA enzymes using a chemical source of sulfide will be discussed². In addition, substrate scope, mechanistic, and structural studies on the YcaO proteins which perform adenosine triphosphate (ATP) dependent peptide backbone activation will be covered³. Finally, the recent discovery of a novel biological sulfur delivery system (TfuA/ThiS) to the designated peptide bond will also be included⁴. These data unequivocally assign a new biochemical function to the YcaO superfamily and the TfuA protein and paves the way for further characterization of new peptide backbone PTMs in natural products and proteins.



References

- 1. N. Mahanta, D. M. Szantai-Kis, E. J. Petersson and D. A. Mitchell, ACS Chem. Biol., 2019, 14, 142.
- 2. N. Mahanta, A. Liu, S. Dong, S. K. Nair and D. A. Mitchell, Proc. Natl. Acad. Sci., 2018, 115, 3030.
- 3. S.-H. Dong, A. Liu, N. Mahanta, D. A. Mitchell and S. K. Nair, ACS Cent. Sci., 2019, 5, 842.
- 4. A. Liu, Y. Si, S.-H. Dong, N. Mahanta, et al., Nat. Chem. Biol., 2021, 17, 585.

An unorthodox synthesis of 2,6-dicyanoaniline and 3-amino-9,10-dihydrophenanthrene-2,4-dicarbonitrile catalysed by potassium 18-crown ether and their *in vitro* study on Calf Thymus DNA

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An efficient two component domino reaction strategy has been developed for the synthesis of 2,6-dicyanoaniline and 3-amino-9,10-dihydrophenanthrene-2,4-dicarbonitrile derivatives in moderate to good yield by the reaction between malononitrile and β -chloro- α , β -unsaturated aldehydes catalyzed by potassium hydroxide-18-crown-6 in methanol. *In vitro* intercalation studies of 3-amino-9,10-dihydrophenanthrene-2,4-dicarbonitriles with Calf Thymus DNA have been carried out which reveal that the moiety interacts with an affinity greater than that of ethidium bromide (EtBr).

Photocatalyst-free visible light mediated denitrative sulfonylation of β-nitrostyrenes using arylazo sulfones

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The photocatalyst-free visible light mediated reactions, based on the presence of a visible light absorbing functional group in the starting material itself in order to exclude the often costly, hazardous, degradable and difficult to remove or recover photoredox catalysts, are gaining momentum recently¹. Simultaneously, denitrative reactions of β -nitrostyrenes have also recently gathered significant attention for the construction of important scaffolds. Vinyl sulfones are one such class of compounds which are widely recognized for their biological activity and synthetic. They have been obtained from β -nitrostyrenes using reagents like sulfinate salts² and sulfonyl hydrazides³ but to the best of our knowledge none of the reports is visible light driven. We have employed the visible light mediated photocatalyst-free approach to develop a denitrative sulfonylation reaction of β -nitrostyrenes employing arylazo sulfones (bench-stable photolabile compounds). Arylazo sulfones served as the sulfonyl radical precursors under blue LED irradiation for the synthesis of (*E*)-vinyl sulfones in dioxane/H₂O 2:1. The absence of any metal, photocatalyst and additive; excellent selectivity (*E*-stereochemistry) and the use of visible light and ambient temperature are the prime assets of the developed method.

References

- (a) Y. Wei, Q.-Q. Zhou, F. Tan, L.-Q. Lu and W.-J. Xiao, *Synthesis*, 2019, **51**, 3021; (b) D. Qiu, C. Lian, J. Mao, M. Fagnoni and S. Protti, *J. Org. Chem.*, 2020, **85**, 12813; (c) R. Chawla, S. Jaiswal, P. K. Dutta and L. D. S. Yadav, *Tetrahedron Lett.*, 2020, **61**, 151898.
- (a) T. Keshari, R. Kapoorr and L. D. S. Yadav, *Eur. J. Org. Chem.*, 2016, 2695; (b) G. Nie, X. Deng, X. Lei, Q. Hu and Y. Chen, *RSC Adv.*, 2016, 6, 75277; (c) G.-F. Hong, J.-W. Yuan, Z.-H. Dong, Y.-M. Xiao, P. Mao and L.-B. Qu, *Phosphorus, Sulfur, Silicon Relat. Elem.*, 2018, 193, 771.
- (a) S. Kumar, R. Singh and K. N. Singh, *Asian J. Org. Chem.*, 2018, 7, 359; (b) T. Yucai, W. Ping, R. Shutong and C. Piao, *Chin. J. Appl. Chem.*, 2019, 36, 664; (c) B. Aegurla and R. K. Peddinti, *Asian J. Org. Chem.*, 2018, 7, 946.

A one-pot fluorogenic cascade cyclization reaction via BF₃-sensing

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Among all boron halides, boron trifluoride (BF₃) which is a non-flammable gas has been mostly exploited as a Brønsted acid plus a Lewis acid on account of its electron deficient character. Regardless of its diverse applications regrettably BF₃ is an extremely corrosive and toxic compound. It has harsh irritant properties for ocular mucous membrane and respiratory airways in animals. As a result, due to rising use of BF₃ as well as its toxic nature toward health and environment, it is crucial to develop a straightforward, scalable, low cost, portable and suitable technique for scrutinizing BF₃. Our aim here to develop a fluorogenic technique where a compound is designed from some inexpensive starting materials to detect BF₃ in elevated sensitivity, fast response rate, unambiguously identifiable colour change etc. (*E*)-3-Phenyl-1-(2-(phenylethynyl)phenyl)prop-2-en-1-one is shown as a chemodosimetric sensor where it selectively senses toxic BF₃, scrutinized through electronic spectral analysis and recognized by the bare eye. Originally the probe is non-fluorescent due to its nonplanar structure. However, after the addition of BF₃ in acetonitrile solution it catalytically reacts with BF₃ and transform to a planner structure through the stepwise



cyclization processes. Ultimately, an innovative compound is structured which is planar and demonstrated an improved fluorescence intensity (60-fold) in less than 2 min along with a extremely low detection limit (6.36×10^{-10} *M*) in the range of 0 to 50 µL exploit it function as a proficient gas phase BF₃ sensor with synchronized detection in a portable form.

References

- 1. M. Mandal, A. K. Mahapatra and A. Kar, *Analyst*, 2021, **146**, 2998.
- 2. S. S. Ali, A. Gangopadhyay, A. K. Pramanik, S. K. Samanta, U. N. Guria, S. Manna and A. K. Mahapatra, *Analyst*, 2018, **143**, 4171.

Reconstitution and mechanistic characterization of the antibiotic promysalin biosynthetic pathway

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Promysalin is a novel antibiotic, isolated from *Pseudomonas putida* which exhibits unique and potent antibacterial activity, most notably against *Pseudomonas aeruginosa*, a notorious opportunistic pathogen in clinical settings in addition to other Gram-negative pathogens¹. Recently, it is also reported to be active against several Gram-positive drug-resistant human pathogens as well, which makes this an interesting broad-spectrum antibiotic². The biological target of promysalin is "succinate dehydrogenase", an enzyme involved both in the tricarboxylic acid cycle and in respiration via the electron transport chain^{3–5}. This amphipathic molecule is composed of salicylic acid and 2,8-dihydroxymyristamide bridged by a unique 2-pyrroline-5-carboxyl moiety. Promysalin is proposed to be assembled from three building blocks: chorismic acid, proline, and myristic acid via an interesting hybridn on-ribosomal peptide synthetase (NRPS) and polyketide synthase (PKS) biosynthetic pathway^{1,3}. Proposed biosynthetic pathway of promysalin include several intriguing enzymatic reactions according to the genetic deletion studies, however, none of these enzymes have been characterized in vitro from the mechanistic and structural standpoint. These include enzymes that activate the three building blocks and assemble them on an NRPS platform (PpgA, PpgJ, PpgC, and PpgL) and the tailoring enzymes such as oxygenase/hydroxylase enzymes (PpgF and PpgN) which carryout regiospecific hydroxylation (C-H activation), PpgO enzyme that perform the terminal amidation and enzymes (PpgB/PpgI) that catalyze the final dehydrogenation reaction to complete the biosynthesis. Current work is focused on understanding the Rieske type hydroxylase (PpgF) which catalyze the regiospecific hydroxylation at C8 of myristic acid using organometallic chemistry, a poorly understood biological enzyme system (non-heme Fe dependent enzyme harbouring [2Fe-2S] cluster as an electron donor). We have successfully cloned and expressed several enzymes on the pathway and efforts are underway for their *in vitro* reconstitution and mechanistic analysis. This study will illustrate the novel chemistry that nature uses to build architecturally complex bioactive molecules and the foundational knowledge on the hybrid PKS/NRPS system will provide the framework for efficient efforts in combinatorial biosynthesis to create library of variants of this broad spectrum antibiotic with possibly novel structures and function.

References

- 1. W. Li, P. E.-D. Santos, S. Matthijs, G.-L. Xie, R. Busson, P. Cornelis, J. Rozenski and R. De Mot, *Pseudomonas. Chem. Biol.*, 2011, **18**, 1320.
- 2. R. D. Kaduskar, G. D. Scala, Z. J. H. Al Jabri, S. Arioli, L. Musso, M. R. Oggioni, S. Dallavalle and D. Mora, *Sci. Rep.*, 2017, **7**, 8861, 1.
- 3. C. E. Keohane, A. D. Steele, C. Fetzer, J. Khowsathit, D. V. Tyne, L. Moynie, M. S. Gilmore, J. Karanicolas, S. A. Sieber and W. M. Wuest, *J. Am. Chem. Soc.*, 2018, **140**, 1774.
- 4. A. D. Steele, K. W. Knouse, C. E. Keohane and W. M. Wuest, J. Am. Chem. Soc., 2015, 137, 7314.
- 5. A. D. Steele, C. E. Keohane, K. W. Knouse, S. E. Rossiter, S. J. Williams and W. M. Wuest, *J. Am. Chem. Soc.*, 2016, **138**, 5833.

Modelled structure of K33-linked diubiquitin and its solution behaviour

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The covalent modification of proteins by ubiquitin is a critical mechanism for propagating signals in cells. The posttranslational modification of proteins with one or several ubiquitin molecules can alter the fate, activity, localization, and protein-protein interactions of the modified protein. Thousands of cellular proteins are modified by ubiquitin and as a consequence, ubiquitylation regulates a wide range of cellular processes in eukaryotes. Seven different type of diubiquitin (Ub) linkages are possible to form chains via isopeptide linkages between the ε -NH₂ group of any of the seven lysines (K6, K11, K27, K29, K33, K48, K63) on Ub and the C-terminus of a second Ub; importantly, all of these linkages are present in the cell at varying levels of abundance. It has been hypothesized that each of these different linkages imparts unique structural and dynamical properties. The solution behaviour for all ubiquitin linkages is more complicated than static crystal structures would suggest. Here we have computed the structure of human K-33 llinkeddiubiquitin and predicted its solution behaviour. We have also computed the solution behaviour of 29-linked diubiquitin. We have already established the methodology to do monoubiquitination by computational approach, we have applied that and modelled the structure of K-33 linked diubiquitin and did molecular dynamic simulation to check the solution behaviour.



A prospective view on chemistry and therapeutic activity of pyrazole: Synthetic strategies and biological applications

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Pyrazole and its derivatives are considered to be very important pharmacologically active scaffolds. On the basis of the literature¹, it has been revealed that good yield (53–95%) can be achieved by chemoselective and regioselective synthesis. Pyrazole under goes electrophilic substitution but nucleophilic substitution is rare one¹. The structural modifications of the basic structure of pyrazole have allowed the preparation of new derivatives with many important structural variations concerning the substituents on the carbon at the 3-position and at the 5-position of the heterocyclic ring which play a crucial role in biologically active compounds and therefore represent an interesting template for combinatorial medicinal chemistry¹. In this particular presentation, the various kinds of synthetic processes for the preparation of pyrazole such as Sonogashira coupling². Michael addition³, Cyclocondensation reaction⁴, Tandem reaction⁴, Vilsmeier-Haack reaction⁵, synthesis of pyrazole by acidcatalyzed imine formation⁶, using 1,3-diols via Hydrogen Transfer Catalysis, Regioselective synthesis of 1,3- and 1,3,5-substituted pyrazoles using diarylhydrazones and vicinal diols and ruthenium(II)-catalyzed intramolecular oxidative CN coupling method⁷ etc. will be reviewed. In this particular presentation, useful advantages like excellent yields, simple workup procedures, non-toxic solvent, environmentally friendly and excellent reactivity of this above mentioned processes will be looked through as a whole. The pyrazole nucleuses have medicinal values such as antibacterial, antifungal, antiviral, antitubercular, anticancer activity etc.⁸. Some of these compounds have also exhibited anti-inflammatory, antidiabetic and analgesic properties⁸. Many pyrazoles have been found to be luminescent and fluorescent agents¹. In the present review, our main interest is to emphasize the various synthetic approaches and chemistry reported by researchers on pyrazole for their various pharmacological activities.

References

- 1. B. De, S. Sen and T. S. Easwari, Asian J. Research Chem., 2012, 5(12), 1483.
- 2. Y. Yang, Z. Hu, Yi. Chen, R. Li and Z. Zhan, Org. Biomol. Chem., 2018, 16, 197.
- 3. V. Sharma, A. Kaur, S. C. Sahoo and S. S. Chimni, Org. Biomol. Chem., 2018, 16, 6470.
- 4. B. Willy and T. J. J. Muller, *Eur. J. Org. Chem.*, 2008, 4157.

- 5. P. Lokhande, K. Hasanzadeh and S. G. Konda, *Eur. J. Chem.*, 2011, 2, 223.
- 6. L. Knorr, *Dtsch. Ber. Chem. Ges.*, 1883, 16, 2597.
- 7. M. J. Naim, O. Alam, F. Nawaj, Md. J. Alam and P. Alam, J. Pharm. Bioallied Sci., 2016, 8(1), 2.
- 8. K. Karrouchi, S. Radi, Y. Ramli and J. Taoufik, *Molecules*, 2018, 23, 134.

A simple and efficient method for the synthesis of biologically relevant aryl- bis(6-aminouracil-5-yl)methane derivatives using mandelic acid as an efficient naturally occurring organocatalyst in water at room temperature

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6-Aminouracil and its derivatives play a key structural part in numerous naturally occurring bioactive compounds, and also regarded as a versatile building block for several nitrogencontaining heterocycles possessing a wide range of pharmacological potentials. In medicinal chemistry, 6-aminouracils are the important starting compounds for the synthesis of xanthenes and theophylline related compounds which are now routinely used as phosphodiesterase inhibitors for the treatment of asthma. After noticing the importance of 6-aminouracils we are also motivated to synthesize these scaffolds under greener pathway.

In continuation of our strong research interest towards organo-catalyzed reactions^{1–3}, herein we wish to report a simple, facile and convenient practical method for the one-pot synthesis of biologically relevant aryl-substituted bis(6-aminouracil-5-yl)methane scaffolds has been developed using mandelic acid as a commercially available and eco-friendly organocatalyst via pseudo three-component condensation reaction between aldehydes and 6-aminouracils in water at room temperature. Mild reaction conditions, use of naturally occurring environmentally benign organocatalyst, water as solvent, good to excellent yields, high atom-economy, environmentally benignity, easy isolation of products, no column chromatographic separation and reusability of reaction media are some of the salient features of the present protocol.

References

- 1. B. Banerjee, Curr. Org. Chem., 2018, 22, 208.
- 2. G. Kaur, K. Bala, S. Devi and B. Banerjee, Curr. Green Chem., 2018, 5, 150.
- 3. G. Kaur, S. Thakur, P. Kaundal, K. Chandel and B. Banerjee, *ChemistrySelect*, 2018, 3, 12918.

Studies on the biosynthesis of bottromycina promising ribosomal antibio

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Ribosomally synthesized and post-translationally modified peptides (RiPP) are a class of natural product have promising biological activities (antibiotic, anticancer etc.). Bottromycin (*Streptomyces bottropensis*) represent a class of heavily modified RiPPs that possesses promising antibacterial activity towards the methicillin-resistant *Staphylococcus aureus* (MRSA) and vancomycin-resistant enterococci (VRE), in addition to other pathogens. It acts by blocking the aminoacyl tRNA binding to the A site of the 50S ribosome, thus inhibiting bacterial protein synthesis, a mode of action that is different than marketed antibiotics. Bottromycins undergo diverse posttranslational modifications on a small core peptide including C-H activation by radical S-adenosylmethionine (radical SAM) enzymes that use [4Fe-4S] cluster, macrocyclization/heterocyclization by adenosine triphosphate dependent YcaO enzymes, and oxidative decarboxylation by cytochrome P450 enzyme, among others. We have recently cloned and expressed radical SAM and YcaO enzymes for performing *in vitro* reconstitution assays to validate their activities, elucidate their substrate scope and characterized them from biochemical and structural studies. In this time of antibiotic resistance, bottromycin holds a great therapeutic promises.

Biological potential of 1,5-benzothiazepine derivatives

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Heterocyclic compounds occur widely in nature and guite a few of these are essential to life processes showing impressive spectrum of physical, chemical and biological properties. In the last few decades, substantial developments in the chemistry of benzothiazepines resulted in a variety of innovative and interesting reactions to construct this moiety and their noteworthy biological potentials. Numerous studies have shown that the benzothiazepine derivatives exhibit wide spectrum of biological activities. The recent studies, aimed to explore the suitability of new hybrid pharmacophore as potential cytotoxic and antimicrobial agents, is taking 1,5-benzothiazepine as an essential nucleus to provide a series of novel compounds. Antibacterial and antiviral activity is one of the most promising features of these derivatives. 1,5-Benzothiazepine derivatives with varying degrees of inhibitory effects on Gram-positive bacteria, Escherichia coli, Staphylococcus aureus and HIV-1 are documented. These compounds also exhibit various therapeutic activities like anti-Inflammatory, anti-cancer, antifeedant, analgesic, anti-convulsant, anti-HIV, calcium antagonists, coronary vasodilators, antidepressant, antihypertensive, ant ischemic, ant arrhythmic, platelet aggregation inhibitor and found useful in mucosal blood flow as antiulcer and gastric secretion inhibitor. Diltiazem and Clentiazem are the first molecules clinically used for their cardiovascular action. Further, Thiazesim, Clothiapine, Seroquel were used clinically for CNS disorders.

The reported general approach for the synthesis of the 1, 5-benzothiazepine moiety is the reaction in between 1,3-diarylprop-2-enones and aminothiophenol. The numerous described methodologies consist of the use of inorganic solid supports such as alumina, silica gel and clay under microwave irradiation, acetic acid or trifluoroacetic acid, hydrochloric acid, piperidine etc.

Interestingly, the flexibility in the methods of their synthesis results in a variety of innovative and interesting reaction to construct this nucleus.

In silico studies, synthesis and anti-tubercular activity of novel heteroaryl functionalized bis-coumarin derivatives

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Tuberculosis, caused by *M. tuberculosis*, has been one of the foremost cause of death worldwide. Till date it is severely widespread due to multi-drug-resistant (MDR) strains as well as drug-resistant (XDR) strains. The mutations in the targets of antibiotics and degradation of antibiotics at the bacterial cell are mainly responsible for evolution of these drug resistant strains. Continuous instances of drug resistance strain of tuberculosis has intensified the urge for finding novel targets that can be inhibited. Mur enzymes are one such effective target, as they are involved actively in the biosynthesis of peptidoglycan which is present in bacterial cell wall and provides rigidity and strength against external environment.

The present study aims to screen a library of unnatural heteroaryl functionalized biscoumarin derivatives using various theoretical tools, to filter active leads having ability to inhibit *Mycobacterium tuberculosis*. Molecular docking studies of these compounds has been performed by using AutoDock 4.2 toolson crystallized structure of Mur enzymes. They have been evaluated further for physicochemical and ADME parameters, to study their molecular properties and bioactivity with different receptors, using molinspiration server and PREADMET server. On the basis of this theoretical exploration, a few potent active leads were filtered and have been synthesized.

Diels-Alder reaction of dibenzazepine and 2,5-dimethylfuran: A DFT study

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The Diels-Alder reaction involving the cycloaddition of dienes and dienophiles is a widely used method for the preparation of six-membered rings. The reaction involves the formation of a product which can have two possible configurations, viz, endo and exo. For a vast majority of the Diels-Alder reactions, endo is the major product. The aim of the present research is to study the feasibility of Diels-Alder reaction between dibenzazepine and 2,5-dimethylfuran by the computational method. The product formed is dehydrated under suitable conditions to give tribenzoazepine. Tribenzoazepine derivatives find a wide variety use in the production of organic light-emitting devices, electroluminescent devices and as intermediates for charge-transporting agents. Computational thermodynamic study of the reaction has been carried out at different temperatures in the gas phase and aqueous medium. Computational parameters show that the reaction is feasible as will be discussed in the oral presentation.

Physical Chemistry Section

[1 - 12]

Physical Chemistry Lecture-1

Towards vibrational tomography of citrate on dynamically changing individual silver nanoparticles

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Trisodium citrate (TSC) has been used in the synthesis of colloidal nanoparticles (NPs) and has probably become the most common reducing and stabilizing agent in the history of noble metal nanomaterials^{1–3}. In this work, we explored changes in binding modes of the most common ligand, citrate on silver nanoparticles (AgNPs) using single-particle surfaceenhanced Raman scattering (SP-SERS). Single AgNPs of 50±10 nm diameter anchored on clean glass slides were monitored using time-dependent SP-SERS with 632.8 nm excitation, at 1.3 μ W incident (0.5 μ W absorbed) power per nanoparticle. We observed several distinct spectra of citrate during time-dependent SP-SERS. Analysis of 1400 spectra showed the



Fig. 1. Laser interacting with citrate-protected AgNPs. SP-SERS measurements resulted in various binding modes and orientations of citrate on individual AgNP.

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existence of two major groups termed as favorable (F) and probable (P) spectra, based on their likelihood of appearance and intensities. These distinct spectra corresponded to a multitude of binding modes, structures, and variants of photocatalyzed products of citrate on the surface of dynamically changing AgNPs. Density functional theory (DFT) simulations were performed to model the structures and binding modes of citrate on an Ag(111) surface and corresponding Raman spectra were computed and compared with distinct spectral types. Experiments performed with deuterated (2,2,4,4-d₄) citrate-capped AgNPs provided additional evidence to understand the shifts in vibrational features obtained in SP-SERS of citrate-capped AgNPs. These systematic analyses of time-dependent SP-SERS spectra may be used for the reconstruction and vibrational tomography (VT) of ligands at the single-particle level. The proposed VT approach is similar to sectioning an object through a multitude of orientations and reconstructing its three dimensional structure, although the structures reconstructed here are molecular orientations.

References

- 1. M. Grzelczak, J. Pérez-Juste, P. Mulvaney and L. M. Liz-Marzán, Chem. Soc. Rev., 2008, 37, 1783.
- 2. I. Ojea-Jiménez, X. López, J. Arbiol and V. Puntes, ACS Nano, 2012, 6, 2253.
- 3. K. Chaudhari, T. Ahuja, V. Murugesan, V. Subramanian, M. A. Ganayee, T. Thundat and T. Pradeep, *Nanoscale*, 2019, **11**, 321.

Physical Chemistry Lecture-2

Molecularly functionalized aminoclays: Versatile materials for new applications

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2D layered materials like natural clays have ordered structures and they provide a direction to develop novel functional materials. Aminoclays (ACs) containing amine groups serve as an attractive class of layered materials with remarkable properties and applications over other natural or synthetic clays. Their interesting properties arise due to the combination of the nanoscopic space within them with the rich surface chemistry of amine groups that are covalently linked to the clay structure. ACs can be incorporated with other material in order to expand their potential. There has been a growing interest in recent years for the development of functional materials using aminoclays. This work explores several aspects of such fascinating materials. We have worked towards the grafting of β -cyclodextrin onto the surface of aminoclay. The as-synthesized AC-CD was shown to be an effective and attractive material for the functionalization of the clay with Ag₂Se@SBB. The interactions between AC-CD and Ag₂Se@SBB resulted in the enhanced luminescence of the clusters. These supramolecular interactions have been studied in detail by various spectroscopic techniques. Aminoclaynylon-6 nanofiber have been developed as "smart surfaces" for desorption electrospray


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ionization mass spectrometry (DESI MS)-based analysis and imprint imaging. The suitability of such nanofiber mats as smart surfaces for DESI MS has been illustrated using specific examples, including patterns formed by single drops with dissolved dyes, marker pen inks, and printing inks. Imprints of plant parts (leaf, flower petal, and rhizome) demonstrated the significance of using aminoclay-nylon-6 nanofiber mats as smart surfaces for identifying and preserving diverse classes of compounds, including aroma and color.

Intense photoluminescence from Cu-doped CdSe nanotetrapods triggered by ultrafast hole capture

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Brightly photoluminescent Cu-doped CdSe nanotetrapods (NTPs) have been prepared by a modified hot injection method. Their photoluminescence (PL) has a quantum yield of 38% and decays slowly over a few microseconds, while the PL in undoped NTPs has a rather small quantum yield of 1.7% and decays predominantly in tens of picoseconds, with a minor component in the nanosecond time regime. PL spectra of doped NTPs are significantly Stokes shifted compared to the band edge (BE). Efficient PL quenching by a hole scavenger confirms the oxidation state of +I for the dopant ion and establishes hole capture by this ion to be the primary event that leads to the Stokes shifted PL. A fast decay of photoinduced absorption band, along with a similar decay in PL, observed in femtosecond optical gating experiment, yields a time constant of about a picosecond for the hole capture from the valence band (VB) by Cu⁺. The remarkably long PL lifetime in the doped NTPs is ascribed to the decrease in the overlap between the wavefunctions of the photogenerated electrons and the captured hole. Hot carrier relaxation processes, triggered by excitation at energies greater than the band gap, leave their signature in a rise time of few hundreds of femtoseconds, in the ground state bleach recovery kinetics. Hence, a complete picture of exciton dynamics in the doped NTPs has been obtained using ultrafast spectroscopic techniques working in tandem.

Isomeric triazine-nLi⁺ (n = 1, 2, 3): Successful exploration in search of hydrogen storage building block

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If hydrogen gas is a suitable name for resolving the energy crisis in the current situation then our studied system Li dopped triazine isomers would be an ideal building block to store hydrogen. All triazine isomers are mono and bi lithiated except 135 triazine which is also tri lithiated and all lithiated triazine isomers are stabilized as a cation. Its well acceptance in the scenario of hydrogen storage material has been justified by stability, reactivity, and aromaticity with the help of hardness (η), electrophilicity (ω), and NICS (0,1) calculations¹. The average adsorption energy varies from 0.60 eV to 0.85 eV, indicating a quasi-molecular type interaction, and topological analysis using the multiwfn package² reveals an ionic type contact between the adsorbing hydrogen and the building block. With considerable gravimetric wt% 10, 17, and 15 respectively, mono, bi, and tri lithiated isomers can adsorb a maximum of 5, 10, and 9 molecular hydrogens. At temperatures of 200 K or lower, hydrogen adsorption occurs spontaneously³.



References

- 1. R. Parida, M. Dash, G. Roymahapatra and S. Giri, J. Indian Chem Soc., 2021, 98, 100065.
- 2. T. Lu and F. W. Chen, Multiwfn, Multiwfn: a multifunctional wavefunction analyzer, *J. Comput. Chem.*, 2012, **33**, 580.
- 3. S. Chattaraj, K. Srinivasu, S. Mondal and S. K. Ghosh, J. Phys. Chem. A, 2015, 119, 3056.

One-pot phosphine-free route for single-component white light emitting CdSeS alloy nanocrystals

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Nanomaterials have emerged as a promising material for white light emitting lighting devices and sensors¹. Commonly, white light is produced by mixing red, green, and blue emitting materials or by mixing two complementary colors in a definite proportion². However, the multi-component systems may lead to possible undesirable changes causing the loss of color purity and decrease in quantum efficiency. Thus, the single-emitting components are advantageous over multiple component systems³. Herein, we report a facile one-pot synthetic route to prepare white light emitting CdSe_xS_y nanocrystals with enhanced quantum yield using cadmium oxide, sulphur powder and selenium powder as starting materials employing a long chain hydrocarbon solvent, paraffin. The phosphine-free solvents are used in the fabrication of the nanocrystals. The optical properties of nanocrystals can be effectively tailored by controlling the reaction time, reaction temperature, and the Se to S molar ratio. The lattice parameters of the crystals were estimated through powder X-ray diffraction (PXRD). The PXRD data revealed that there is linearity in the lattice parameter which indicates the



Fig. 1. The schematic illustration of the properties and application of the white light emitting nanocrystals.

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homogeneous alloy of the nanocrystals on changing the molar ratio of Se to S⁴. The emission of pristine CdSe_xS_y nanocrystals can be tuned across the visible region by changing the molar ratio of Se to S. The band-edge and trap-state emission were observed covering a whole visible range leading to a single-component white light emission was observed. The longer wavelength emission was found to be originated through trap states. The fine-tuning of the composition and the reaction time led to the efficient generation of the white light emitting dispersion with Commission Internationale de l'Eclairage (CIE) coordinates of (0.30, 0.31). The white light emission of the nanocrystals can be retained in the hydrogel matrix and polymer-embedded thin films with CIE coordinates (0.31, 0.32) and (0.31, 0.33), respectively. The color rendering index (CRI) and correlated color temperature (CCT) of CdSe_xS_y nanocrystals embedded polymer thin films were 95 and 6453 K, respectively⁵. High CRI and suitable CCT values hold promise for solid-state lighting devices.

References

- 1. S. Jaiswal, S. Kundu, S. Bandyopadhyay and A. Patra, Nanoscale Adv., 2021, 3, 3232.
- 2. S. Kundu, B. Sk, P. Pallavi, A. Giri and A. Patra, Chem. Eur. J., 2020, 26, 5557.
- T. Rosson, S. Claiborne, J. McBride, B. Stratton and S. Rosenthal, J. Am. Chem. Soc., 2012, 134, 8006.
- 4. O. Adegoke, M. Seo, T. Kato, S. Kawahitob and E. Park, J. Mater. Chem. B, 2016, 4, 1489.
- 5. S. Jaiswal, J. Pathak, S. Kundu and A. Patra, ACS Sustainable Chem. Eng., 2021, 9, 5613.

Deciphering the evolution of supramolecular nanofibers in solution and solid-state: A combined microscopic and spectroscopic approach

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Supramolecular self-association of small π -conjugated organic molecules leads to welldefined nanoarchitectures like vesicles, micelles, low molecular weight gels, and other noncovalent aggregates¹. Such molecular aggregates have been explored for different applications ranging from bioimaging to sensors and switches². In this context, aggregates of heteroaromatic thiophene-based donor-acceptor molecules capture the significant attention due to the size and morphology-dependent tunable emission³. However, the correlation between the nature of the morphology (solid-state characterization) and the emission behaviour (dispersion-state analysis) of the aggregates are often rudimentary and can be benefitted through further analysis. In this present study, we demonstrated the detailed insight of the nanofiber evolution from a true solution for a thiophene-based acceptor- π -donor- π acceptor molecule (TPAn) through steady-state absorption, emission, electron microscopy, and fluorescence correlation spectroscopy (FCS) analysis. The field emission scanning electron microscopy (FESEM) images showed the formation of the connected network of nanofibers for the dispersion having water content 80%. However, the formation of smallersized nanofibers in the dispersion was realized from FCS results (Fig. 1)⁴. Such smaller nanofibers can be transformed into the connected network of nanofibers through agglomeration during the solvent evaporation in the course of sample preparation for the electron microscopy (Fig. 1)⁴. Besides, the self-assembly of TPAn was explored in the complex and heterogeneous medium, like HeLa cells, revealing the contrasting optical responses in lipid droplets compared to that in the bulk solution and molecular aggregates. Hence, we believe the present study will provide a general experimental protocol to establish the relation between the nature of morphology and emission behaviour for all-organic fluorescent nanoaggregates.



Fig. 1. Schematic illustration depicting the evolution of nanofibers from true solution through electron microscopy coupled with fluorescence correlation spectroscopy (FCS). The role of pyridinic nitrogen centre for the nanofiber formation was also demonstrated using FCS and molecular modelling studies.

References

- 1. G. M. Whitesides and B. Grzybowski, *Science*, 2002, 295, 2418.
- (a) S. Kundu, B. Behera, A. Giri, N. Saha and A. Patra, *Chem. Commun.*, 2021, **57**, 6875; (b) S. Kundu, B. Sk, P. Pallavi, A. Giri and A. Patra, *Chem. Eur. J.*, 2020, **26**, 5557; (c) V. Kumar, B. Sk, S. Kundu and A. Patra, *J. Mater. Chem. C*, 2018, **6**, 12086;
- 3. X. Zhang, Z. Chen and F. Würthner, J. Am. Chem. Soc., 2007, 129, 4886.
- 4. S. Kundu. A. Chowdhury, S. Nandi, K. Bhattacharyya and A. Patra, Chem. Sci., 2021, 12, 5874.

Adiabatic switching among quantum dot eigenstates: Role of anharmonicity and noise

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In the present study we inquires into the time-dependent quantum adiabatic switching (TDQAS) among the quantum dot (QD) eigenstates under the approval of Gaussian white noise (GWN) with special emphasis on anharmonicity that may be present in the QD potential. The initial and the final eigenstates are distinguished by different values of magnetic field strength, confinement potential, anisotropy and anharmonicity. The QAS has been conducted using four different switching functions (SFs) e.g. square, exponential, sinusoidal and logarithmic. The time-development of switching has been minutely monitored with the help of overlap function and quantum information entropy (QIE). The switching paths have been found to be possessed with features like enhancement, depletion, maximization, minimization and crossover of the overlap function and entropy. These characteristics of the switching paths depend on presence/absence of noise, its pathway of application (additive/multiplicative) and symmetry (odd/even) of the anharmonic potential. The study merits importance in view of vast technological applications of QD-based systems where the noise-anharmonicity interplay may be utilizeded to a great extent.

References

- 1. I. Karabulut and S. Baskoutas, J. Appl. Phys., 2008, 103, 073512.
- 2. J. M. Leonora and A. J. Peter, Solid State Commun., 2010, 150, 30.
- 3. C. A. Duque, N. Porras-Montenegro, Z. Barticevic, M. Pacheco and L. E. Oliveira, *J. Phys. Con*densed Matter, 2006, **18**, 1877.
- 4. P. Sarkar, S. Adhikari and S. P. Bhattacharyya, Chem. Phys., 1997, 215, 309.
- 5. A. Ghosh, A. Bera, S. Saha, S. M. Arif, M. Ghosh, *Superlattice Microst*, 2018, 114, 259.

Effect of antidepressants drugs on micellization behaviour of cationic surfactants: A physicochemical approach

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The influence of antidepressants drugs i.e. chlorpromazine hydrochloride (CPZ) and promethazine hydrochloride (PMZ) on micellization behaviour of cationic surfactants tetradecyltrimethyl ammonium bromide (TTAB) have been investigated using surface tensiometer, conductivity meter, fluorescence and dynamic light scattering (DLS) measurements. Different interfacial and thermodynamic parameters have been calculated by surface tensiometer and conductivity measurements, respectively. Further, the aggregation behaviour (N_{agg}) and Stern-Volmer quenching constant (K_{sv}) has been evaluated using fluorescence spectroscopic technique. The size of micellar aggregates of TTAB in presence of drugs has been measured by DLS. This study conclude that the CMC of pure surfactants decreases in the presence of different concentration of drugs.

Studies on micellar properties of Gemini surfactant in the presence of oxime-functionalized ionic liquid

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The interfacial and thermodynamic properties of two Gemini surfactants i.e. alkanediyi- α,ω -bis(dimethylhexadecyl ammonium bromide) (16-*s*-16, where *s* = 10, 12) have been studied in the presence of an oxime based ionic liquid (IL) i.e. 4-((hydroxyimino)methyl)-1-(2-(octylamino)-2-oxoethyl)pyridin-1-ium bromide (4-PyC8) IL in aqueous solution using surface tensiometer, conductometer, fluorescence, FTIR and ¹H NMR spectroscopic techniques. It has been observed that CMC of Gemini surfactants is decreased on addition of IL, thus, facilitating the micellization process. The various thermodynamic parameters and interfacial properties was evaluated by using conductivity and surface tension measurement, whereas, aggregation number and Stern-Volmer constant were evaluated by fluorescence measurement technique. The ¹H NMR spectroscopic was applied to investigate the interaction between Gemini surfactants and IL to confirm the binding interaction between them. Further, the interaction of antidepressant drugs promethazine hydrochloride (PMZ) with 4-PyC8 IL is studied within Gemini micellar solution.

Electrochemical synthesis of urea by co-reduction of $\rm N_2$ and $\rm CO_2$ under ambient conditions

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Urea is synthesized industrially in two steps $[N_2 + H_2 = 2NH_3 \text{ and } NH_3 + CO_2 = CO(NH_2)_2]$ which requires high temperature and pressure hence an expensive and environmentally hazardous process. We have developed an electrochemical strategy to produce urea in a single step at normal temperature and pressure.

In our work we present a single molecule possessing multiple active sites responsible for dual reduction of N₂ and CO₂ gases to produce urea. The copper phthalocyanine nanostructure owing to its multiple active sites namely the metal center, pyrrolic nitrogen and pyridinic nitrogen plays the key role of potential electrocatalyst which in turn produces urea yield rate of 144 μ g h⁻¹ mg⁻¹ cat and Faradic efficiency of 13% at –0.6 V vs RHE using 0.1 *M* KHCO₃ as an electrolyte.

Solvent mediated electron-phonon relaxation dynamics in core-shell Au-SiO₂ nanoparticles

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Relaxation dynamics of surface plasmons in core-shell Au-SiO₂ nanoparticles have been followed by femtosecond pump-probe technique^{1,2}. The effect of excitation pump energy and surrounding medium on the time constants associated with the hot electron relaxation has been elucidated. A gradual increase in the electron-phonon relaxation time with pump energy is observed and can be attributed to the higher perturbation of the electron distribution in AuNPs at higher pump energy³. Variation in time constants for electron-phonon relaxation in different solvents is rationalized on the basis of their thermal conductivities, which govern the rate of dissipation of heat of photoexcited electrons in the nanoparticles⁴. On the other hand, phonon-phonon relaxation is found to be much less effective than electron-phonon relaxation associated with it remain unaffected by thermal conductivity of the surrounding solvent.

References

- 1. L. Wang, T. Rossi, M. Oppermann, B. Bauer, L. Mewes, D. Zare, T. H. Chow, J. Wang and M. Chergui, *J. Phys. Chem. C*, 2020, **124**, 24322.
- T. Stoll, P. Maioli, A. Crut, S. Rodal-Cedeira, I. Pastoriza-Santos, F. Vallée and N. Del Fatti, *J. Phys. Chem. C*, 2015, 119, 12757.
- M. B. Mohamed, T. S. Ahmadi, S. Link, M. Braun and M. A. El-Sayed, *Chem. Phys. Lett.*, 2001, 343, 55.
- M. Hu, X. Wang, G. V. Hartland, V. Salgueiriño-Maceira and L. M. Liz-Marzán, *Chem. Phys. Lett.*, 2003, 372, 767.

Solvation dynamics in solvent free protein – polymer surfactant biomolecular assemblies

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Solvent-free proteins have attracted tremendous attention in recent times, due to its potential use as a green, nonaqueous solvent with low-volatility, for the synthesis of organic and inorganic compounds, as electrolytes, catalysis, etc.^{1,2}. While dynamics of dye-labelled HSA has been reported³, we focus on solvation dynamics of solvent-free protein, labelled with CPM (7-dimethylamino-3-(4-maleimidophenyl)-4-methyl-coumarin) dye to understand bound water dynamics. This study has been done using fluorescence correlation spectroscopy (FCS) with a conformational dynamics model of data analysis and a comparative examination of hydrodynamic radii of different CPM labelled HSA modified systems. Solvent free causes blue shift in the emission maxima from CPM covalently bound to HSA. In the present experiment, the conformational relaxation time of solvent free CPM labelled HSA is found to increase, while solvent response around the protein is ultraslow.

References

- 1. A. Mukhopadhyay, T. Das, A. Datta and K. P. Sharma, *Biomacromolecules*, 2018, **19(3)**, 943.
- 2. A. P. S. Brogan, K. P. Sharma, A. W. Perriman and S. Mann, Nat. Commun., 2014, 5, 1.
- 3. D. K. Sasmal, T. Mondal, S. Sen Mojumdar, A. Choudhury, R. Banerjee and K. Bhattacharyya, *J. Phys. Chem. B*, 2011, **115(44)**, 13075.

Applied Chemistry Section

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Diclofenac, a "old friend" of pain relief as a modern repurposed weapon of cancer therapy

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Diclofenac is one of the prominent members of non-steroidal anti-inflammatory drugs (NSAIDs), routinely used as normal pain killer for its anti-inflammatory, analgesic and antipyretic activities. "Drug repurposing" is a newly emerging concept to treat a broad range of diseases worldwide. Modern research claims that some of the so called 'old drugs' can be prescribed to treat other diseases in addition to the clinical conditions they are generally used for. The search for new drugs for treating cancers needs huge amount of time, financial investment and manpower involvement. Moreover, drugs need to cross various hurdles like clinical trials for final approval. Our preliminary results establish that besides anti-inflammatory activities Diclofenac is able to introduce antimitotic effect in HeLa (a cervical cancer cell line) with an IC₅₀ concentration (50% inhibitory concentration) 175 uM. It induces cell death mainly via apoptosis, a programmed cell death method. Diclofenac introduces cell death by inhibiting the enzymatic activity of Lactate dehydrogenase A (LDH-A) which is a key enzyme involving in energy production (ATP generation) in cancer cell in hypoxic condition. Molecular docking study with Diclofenac and LDH reveals preliminary interaction that has been substantiated through spectroscopic binding studies between the drug as well as with LDH. Validation of new cellular targets of Diclofenac might qualify it as a future lead compound in the development of anticancer agents delineating repurposed Diclofenac with a novel role in eukaryotic system.

Chemistry of food preservatives

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Recently people are very much using fast food, packaging food, cosmetics etc. As a result, obesity, much non-curable disease like cancer is increasing day by day. Preventable Cancer is still now beyond our hand. Other diseases are curable, but it brings always bitter test to our life. We used to take the meat, colored vegetables from the market. So in these days food additives are an important and thinkable chapter to us. We don't know which of the above disease comes to our life as slow poison from food, from our daily diet. So this work is for conscious of those people who used to take food from outside or use packaging food and be aware for the coming days.

A photocatalytic approach in Medicinal Chemistry for synthesis of 1,2,3-triazole compounds of pharmatceutical/biological importance

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Manufacturing of essential organic compounds like pharmaceutical products/medicines, pesticides, food additives to name a few is a crucial practice and business of everyday life. Over the years chemical companies have been following standardized procedures. However aradually with advent of technologies and awareness in respect to environmental impact, we have come to know that such processes are hazardous and non-environmental friendly. Also it has been realized that such conventional methodologies often involve harsh operating conditions (high temperature and pressure) and at the same time are not cost-effective. As a result the global inflation of daily medicine and other pharmaceutical compounds have become a crucial problem for economic sustainability. Therefore, scientists across the world have started to develop alternative green and new methodologies for synthesizing value added and commercially important organic molecules/compounds. Amongst limited possibilities, a very promising methodology attracting the scientific community is the utilization of photocatalysts in synthesizing desired and specific compounds in presence of light. The beauty of heterogeneous photocatalytic organic synthesis (HPOS), is in involvement of minimum reaction steps and also possibility of carrying out one-pot synthesis. Photocatalysts are generally nanosized semiconductors with narrow band gaps. The specialty of these catalysts is that they are capable of carrying out oxidation and reduction reaction at the same time and hence can be utilized for organic synthesis. Photocatalytic system of synthesis is green, cheaper and also energy harvesting. With advancement in research in this particular field, targeted synthesis and controlled reaction outcome can be achieved with alteration in solvent, catalyst surface property, inducing surface defects and using multi-catalyst systems.

As a part of our continuing research in new methodology development for synthesis of triazolyl organic compounds of biological and pharmaceutical importance, we decided to explore the field of photocatalytic triazolyl click chemistry. It is well known that triazole compounds containing three nitrogen in the five-membered aromatic azole ring are potential clinical drug candidates. Large numbers of triazole compounds have been used as anticancer,

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antipyretic, antidiabetic, antiparasitic etc. drugs commercially. Hence in the present work we have designed and synthesized novel Cu(II) doped TiO₂ nanocomposite for carrying out 1,2,3-triazolyl click reaction in green solvent, absence of base with excellent turnover number, high yield, fast reaction kinetics. Upon light irradiation ($\lambda = 400$ nm), the TiO₂ nanocore releases electron from its valence band to the conduction band which in turn photochemically reduces Cu(II) to Cu(I), achieving spatial and temporal control over the CuAAC reaction. We also address the role of the hole and oxygen in air as a green oxidant, which possibly maintains the Cu(I) to Cu(II) catalytic cycle as feed for the photocatalyst. The new catalytic system is tolerant to air, wide range of substrates/functional groups, uses green solvent and thus advantageous over other reported catalytic systems.

Sensing of Vitamin C and toxic metal ions using green synthesized silver nanoparticles obtained from plant extract

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An eco-friendly approach for the green synthesis of silver nanoparticles (AgNPs) by the reduction of silver ions (Ag⁺) using *Murraya koenigii*(*Mk*) leaf extract has been employed here. Synthesized AgNPs were fully characterized by Ultraviolet-visible (UV-Vis) absorption spectroscopy, Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), dynamic light scattering (DLS), high-resolution transmission electron microscopy (HRTEM) and energy dispersive X-ray (EDX) studies. AgNPs would exhibit surface plasmon resonance (SPR) band at 402 nm. FTIR studies confirmed the presence of different biomolecules responsible for the stabilization as well as formation of AgNPs. HRTEM and DLS techniques were utilized to determine surface morphologies and size distribution of synthesized AgNPs, respectively. The average particle size was found in the range of 5–35 nm. XRD analysis confirmed the formation of face-centered cubic (FCC) crystalline lattice of AgNPs. Presence of elemental silver (Ag) was confirmed by EDX studies. AgNPs exhibited SERS activity that could effectively sense Vitamin C. AgNPs were further utilized for the detection of different heavy and transition metal ions.

Study of morphological and electrochemical properties of (acrylonitrileco-2-acrylamido-2-methyl-1-propanesulfonic acid) conetwork cation exchange membranes

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Homogeneous crosslinked conetwork cation exchange membranes (CEMs) were synthesised by sequential reaction of hydrazine hydrate and nitrile moieties of random copolymers of poly(acrylonitrile) and poly(2-acrylamido-2-methyl-1-propanesulfonic acid) (PAN-*co*-PAMPS). The crosslinked membranes were prepared from the copolymers (PAN-*co*-PAMPS) of varying AN to AMPS mol ratio. Copolymerization of the two monomers enhances miscibility between relatively hydrophobic PAN and hydrophilic ionic PAMPS domains which prevents microphase separation in the membrane matrices. DSC, DMA, TEM, and AFM analyses confirmed the homogeneous phase morphology of the membrane matrices. Both crosslinked (conetwork) and un-crosslinked copolymers (different composition) acted as CEMs. The CEMs were employed for desalination via electrodialysis.



(A) DSC curves of the crosslinked and un-crosslinked membranes, (B) storage modulus vs temperature.

Ultra thin nickel oxide nanosheets having highly exposed Ni³⁺ dopped high energy {110} facets for catalytic application

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Ultrathin NiO (Nikel Oxide) nanosheets with high surface-energy facets are gaining attention, owing to their excellent catalytic property. Two-dimensional NiO nanocrystals generally possess a large lateral size and thickness exhibit a lack of coordinatively unsaturated active/reactive edge and corner sites, which can adversely affect their properties. In this study, round-ultrathin NiO nanosheets (diameter \approx 60–300 nm, thickness <10 nm) were synthesized using a hydrothermal method followed by calcination. Upon increasing the concentration of NaOH in the medium, the sizes of these nanosheets increased without any change in their thickness. The nanosheets were characterized via powder-XRD, field-emission scanning electron microscopy, high-resolution transmission electron microscopy (HRTEM), and selected area electron diffraction (SAED) analysis. HRTEM and SAED revealed that these NiO nanosheets mainly comprised an exposed high-energy {110} surface. XPS analysis revealed that an unsaturated Ni³⁺ site was present in the NiO nanosheets. The NiO nanosheet exhibited high catalytic activity for the aromatic-aldehyde reduction reaction.

The effects of zirconia nanoparticles on crystallization and biological behaviour of bioactive glass ceramics

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The development of glass-ceramics materials for biomedical purposes significantly increased in recent decades. A bioactive glass-ceramics (BGC) has a specific biological response at the implant interface, resulting in forming a strong bond between implant material and tissue. The biomaterials used as bone substitutes, besides being bioactive, should provide adequate mechanical properties similar to that of bone tissue. Zirconia-containing bioactive glass-ceramics (ZBGC) have been accepted as trusting bone implants in clinical applications due to their chemical stableness, high mechanical properties, and hydroxycarbonate apatite (HCA) formation capability.

The objective of the present study is to investigate the effect of crystallization, surface morphology, and biological behaviour of glass-ceramics containing $CaO-AI_2O_3-SiO_2-P_2O_5-CaF_2$ -nanoZrO₂ system in order to advance the development of new bone substitutes. Therefore, as-prepared bioactive glass-ceramics were first examined by the differential thermal analyzer (TG/DTA), X-ray difraction (XRD) analysis, scanning electron microscopy (SEM), and Fourier transform infrared spectrum (FTIR) to characterize all samples. Micro Vicker's hardness test was carried out to investigate the mechanical properties of nano zirconia containing bioactive glass-ceramics. The biological behaviour was evaluated by *in vitro* test. MTT assay and antibacterial activity studies were carried out to confirm the accuracy of the results of the biological evaluation.

Porous organic polymers for size and charge selective sequestration of organic micropollutants from water

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Organic micropollutants are a diverse set of analytes including pesticides, pharmaceuticals, toxic dyes, and plastic precursors which pose a serious threat to human health and aquatic lives¹. Sorption is one of the most energy-efficient techniques to purify water from micropollutants. Porous organic polymers (POPs)², owing to excellent hydrothermal stability, heteroatom decorated tunable pores and high surface area have emerged as advanced adsorbent materials for the efficient removal of micropollutants from water¹. Our group has



Figure. Schematic representation of the removal of the broad-spectrum organic micropollutants from water by porous organic polymers (POPs).

come up with unique design strategies for the development of scalable POPs for sustainability and environmental remediation³. In this presentation, I shall discuss the triptycene-based hypercrosslinked POPs with distinct nanoscale morphologies (irregular aggregates, nanospheres, and nanosheets) for the ultrafast (within 30 s) sequestration of broad-spectrum persistent organic micropollutants from water and delineate the morphology-activity correlation⁴. Addressing the selectivity issue for micropollutant separation, I shall move to the cavitand-based POP discussing the importance of guest responsive resorcin⁴ arene cavitand as a building unit for the size-selective charge-specific separation of organic micropollutants from water⁵.

References

- 1. A. Alsbaiee, B. J. Smith, L. L. Xiao, Y. H. Ling, D. E. Helbling and W. R. Dichtel, *Nature*, 2016, **529**, 190.
- 2. (a) A. G. Slater and A. I. Cooper, *Science*, 2015, 348, 6238.
- 3. (a) S. Bandyopadhyay, S. Kundu, A. Giri and A. Patra, *Chem. Commun.*, 2018, **54**, 9123; (b) M. W. Hussain, V. Bhardwaj, A. Giri, A. Chande and A. Patra, *Chem. Sci.*, 2020, **11**, 7910; (c) A. Giri, N. N. Patil and A. Patra, *Chem. Commun.*, 2021, **57**, 4404.
- 4. A. Giri, S. Biswas, T. K. Dutta, M. W. Hussain and A. Patra, Chemrxiv, doi:10.26434/ chemrxiv.14333936.v1.
- 5. A. Giri, M. W. Hussain, B. Sk. and A. Patra, *Chem. Mater.*, 2019, **31**, 8440.

Elimination of Methylene Blue from synthetic medium by adsorption using acid-treated Bamboo leaves

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In the present study, H_3PO_4 treated bamboo leaves (PBL) are used as a bio-adsorbent to remove Methylene Blue (MB) in the batch process. The effects of different operating parameters like pH (2–10), adsorbent dose (1–10 g.L⁻¹), contact time (5–360 min), and temperature (298–318 K) on the bio-adsorption of MB were reported. The experimental data follows the pseudo-second order model and the Langmuir isotherm. Hence, the process is monolayer adsorption process. The maximum bio-adsorption capacity is 90 mg.g⁻¹ was achieved. Hence, it can be concluded that acid treated bamboo leaves have been utilized as a biosorbent for MB.

Removal of Malachite Green using bamboo leaves: Adsorption study and semi-empirical quantum chemical calculations

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In the current investigation, bamboo leaves (BL) were utilized as adsorbents to eliminate Malachite Green (MG) from the synthetic medium. The adsorption study was executed under the variation of different experimental conditions like pH (2-8), adsorbent dosage (1-10 g/ L), the contact time (5–300 min), and the temperature (298–318 K) on the MG. The $q_{\rm max}$ of adsorption, i.e. 98 mg/g, was achieved for BL. The Redlich-Peterson isotherm model (R^2 = 0.99) fitted appropriately with the experimental data under a specified range of initial concentrations of MG (10-300 mg/L). In the kinetics study, the pseudo-second order model $(R^2 \ge 0.99)$ was revealed as a best fitted model, indicating that adsorption is controlled by chemisorption. The FTIR, Raman spectra, and ¹³C NMR results show that different functional groups of cellulose, hemicellulose and lignin are involved in MG elimination. The theoretical studies were applied for a deeper understanding of the adsorption mechanism of MG using semi-empirical quantum chemical calculations. The semi-empirical quantum chemical calculations also yielded valuable data about quantum chemical properties such as E_{HOMO}, ELIMO, electrophilicity, chemical reactivity, dipole moment, and hardness for adsorbent/ adsorbate components present in bamboo leaves and the binding energy from adsorbent/ adsorbate interactions.

Synthesis and characterization of novel lithium-releasing bioactive glass for biomedical application

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Bioactive glass and glass-ceramics have emerged as an important class of biomaterials because of their ability to bond to hard and soft tissues and release therapeutic ions, which can stimulate neighboring cells. Biomedical applications of these biomaterials range from bone-implant and bone grafts, tissue engineering to drug delivery^{1–3}. Lithium ion has been found to control the Wnt/ β -catenin cell signaling pathway, which is one of the primary factors in generating and repairing hard tissues in bone and teeth⁴. So, bioactive glass that releases lithium ions can potentially regulate the formation of hard tissue. The present work deals with the synthesis and characterization of a novel bioactive glass containing lithium as the therapeutic agent in the glass composition. The composition of the 4 glass samples synthesized was 45 SiO₂.xLi₂O.(25-x) Na₂O.16 CaO.4 P₂O₅.5 MgO.5 B₂O₃, all amounts in wt%, with x being 0, 5, 15, and 25.

The glass density decreased with increasing lithium % due to lower molecular weight compared to sodium. FTIR spectra exhibited the characteristic Si-O-Si glass network, and the XRD data confirmed the amorphous nature of all 4 glass samples. The DTA analysis showed good thermal stability with a glass transition temperature (T_g) ranging from 620 to 650°C. The *in vitro* bioactivity was tested by soaking in SBF solution for 7 days and then analyzing SEM, FTIR and XRD data to confirm the formation of the surface hydroxyapatite layer. All the glasses were found to be bioactive. The cytotoxicity of the glasses was assessed by using human Carcinoma A549 and *E. coli*, where no cell death or growth inhibition was observed, thus, confirming the non-toxic nature of the glass samples. So, it can be concluded that the synthesized bioactive glass can be considered a potential candidate for bone and dental applications.

References

- L. L. Hench, in: "Fundamental Aspects of Biocompatibility", ed., D. F. Williams CRC Press, Boca Raton, Florida, 1981, p. 67.
- 2. L. L. Hench, J. Am. Ceram. Soc., 1991, 74(7), 1487.
- 3. L. L. Hench and J. K. West, Life Chem. Rep., 1996, 13, 187.
- 4. H. Clevers, K. M. Loh and R. Nusse, Science, 2014, 346, 54.

Adsorptive removal of organic dye from aqueous solution with and without nanocomposite adsorbent – A comparative study

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Water pollution due to excessive load of heavy metal and organic dyes becomes a severe environmental issue. Heavy metals and dyes can be removed easily by adsorption using solid adsorbents from wastewater. Adsorption is an economically most favorable process in third-world countries. The adsorption capacities of synthetic adsorbents are more significant than that of agricultural and industrial wastes.

Chitosan and chemically modified chitosan have been used to remove heavy metals and organic dyes from wastewater over the years. Chitosan nanocomposites show a potential role in the adsorption of heavy metals and dyes due to increased chemical stability and adsorption capacity of the adsorbents. Titania-based materials can be applied for the adsorption of various pollutants.

The present study deals with the preparation and characterization of chitosan-nTiO₂ nanocomposites. Different adsorbent samples were prepared with the different weight ratios of chitosan to nTiO₂. The adsorption capacity of the prepared adsorbents towards Methylene Blue dye in an aqueous solution was also investigated. The adsorption experiment was conducted in batch mode under varying experimental conditions such as different pH values, initial metal ion concentration, adsorbent dosage, temperature, and contact time. Various isotherm and kinetic models are tested with the experimental data, and thermodynamic conditions required for adsorption are also calculated. The possible mechanistic pathway of the adsorption process is also discussed.

Biosorption of Ni²⁺ by Ni²⁺ resistant *Saccharomyces cerevisiae* in the presence of some vitamins

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Ni(II) biosorption from an aqueous solution using 5000 mg/L Ni²⁺ resistant S. cerevisiae in the presence of different vitamins is reported. The Saccharomyces cerevisiae (native) biomass was procured and isolated from Kothari Fermentation and Biochem Ltd., [KFBL.BO] Saket, India. Then with the native biomass, 5000 mg/L Ni²⁺ resistant Saccharomyces cerevisiae has been prepared in the laboratory by progressively increasing nickel concentration (Nickel sulfate heptahydrate) in S. cerevisiae growth medium from 500 to 6000 mg/L. Then pour plate technique was applied to isolate the single resistant colony of 5000 mg/L resistant S. cerevisiae as the MIC is 5500 mg/L. Molecular characterization and physical characterization have been performed of Ni²⁺ resistant S. cerevisiae, such as SEM-EDS and FTIR. Vitamins are essential nutrients for cellular growth, having antioxidant activity but become toxic at higher concentrations. The vitamins are added in the fermentation broth with varying concentration of 0.05–1.5 μ g/mL and its effect on the biosorption capacity are investigated. The Ni(II) biosorption was decreased with biotin, riboflavin, nicotinic acids, vitamininositol, Ca-D pantothenate but increased with L-ascorbic acid, folic acid, pyridoxine hydrochloride, thiamine hydrochloride, at concentration 0.1 µg/mL, and for L-ascorbic acid, the concentration is 0.03 μ g/mL. The maximum biosorption removal obtained is 95% by Lascorbic acid, 93.2% by pyridoxine hydrochloride, 92.2% by folic acids, and 88.4% by thiamine hydrochloride, which gave a much positive impact on Ni(II) biosorption.

Synthesis of ashwagandha extracts loaded chitosan-pectin biocomposite films for biomedical applications

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Nowadays, natural products (polymers, clays, proteins, plant extracts) received a great attention of researchers and are considered the most important components to be used in biomedical applications. Chitosan is a polycationic linear, carbohydrate polymer derived by alkaline deacetylation of chitin. Chitin is found in sea animals such as crabs, shrimps, and lobsters to name a few. It possesses good film forming ability, biocompatibility, biodegradability, hemocompatibility, non-toxicity, and antibacterial activity¹. Pectin is also a carbohydrate polymer containing galacturonic acid units. It is widely used in food industry and pharmaceutical applications^{2,3}. In this study, chitosan (CS) and pectin (P) based biocomposite films loaded with natural extracts (root and leaf) of ashwagandha were fabricated through solvent casting method. The prepared biocomposite films were characterized by various physicochemical and biological parameters. The prepared biocomposite films were transparent, hemocompatible, and biodegradable with high water holding capacity and good flexibility. On the basis of above mentioned properties, it was concluded that ashwagandha extracts loaded chitosan-pectin biocomposite films could be used as suitable candidate for biomedical applications such as wound healing.

References

- 1. N. Devi and J. Dutta, Asian Chitin J., 2015, 11, 1.
- 2. R. Chacón-Cerdas, A. Medaglia-Mata, D. Flores-Mora, et al., Chem. Pap., 2020, 74, 509.
- 3. L. Neufeld and H. Bianco-Peled, Int. J. Biol. Macromol., 2017, 101, 852.

In vitro and *in silico* analysis of a dihydropyridine derivative (Amlodipine besylate) as an anti-cancer drug: Microtubule targeting agent

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Microtubules have been recognized as a highly attractive target for anti-cancer drugs. A number of compounds such as paclitaxel, vinblastine and colchicine exert their effect by altering the dynamics of microtubules. We report the mechanism of action of Amlodipine besylate (AB) which is a synthetic derivative of a dihydropyridine drug Amlodipine, as an anti-cancer agent. The effect of AB on apoptosis in HeLa human cervical cancer cells and the apoptosis associated signaling pathways were determined using various methods, including cell viability assay, Annexin V/Propidium iodide (PI) staining, mitochondrial membrane potential ($\Delta \psi m$) assay, reactive oxygen species (ROS) assay and western blot analysis. On basis of *in vitro* test, AB demonstrated a dose dependent cytotoxic effect against HeLa cells and early apoptosis occurred when the cells were treated with 10 µM AB. Furthermore, AB treatment induces loss of $\Delta \psi m$ potential, increased ROS production, downregulated procaspase3 which indicates that AB potentially acts via the intrinsic apoptotic signaling pathway. Confocal microscopy showed that AB alters the microtubule architecture of HeLa cells. AB has been confirmed as a colchicine binding site inhibitor (CBSI) using AutoDock Vina 4.2 program. AB exhibited highest binding free energies for CBS in comparison to taxol, vinblastine and laulilamide binding domain. The derivative binds tubulin in a similar manner to colchicine by establishing two hydrophobic interactions with LYS³⁵², ALA³¹⁶, hydrogen bonding with CYS²⁴¹ and a pi-sulfur bond with MET²⁵⁹ at the binding pocket. The results indicated that AB can be a promising inhibitor of tubulin polymerization for the treatment of cancer.

Large scale synthesis of metal phthalocyanine nanostructures: Efficient electrocatalyst for ammonia synthesis under ambient conditions

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Ammonia synthesis by electrochemical nitrogen reduction reaction (ENRR) at ambient conditions can substitute the century old Haber-Bosch process; which results in global 2% carbon dioxide emissions annually. However the ENRR process suffers poor yield rate of ammonia and lower Faradic efficiency. Thus the solution lies in the design of specific active site generation of the electrocatalyst for enhanced ENRR performance. Herein, we demonstrate metal phthalocyanine (MPc) nanostructure having well-defined MN₄ configuration as a model electrocatalyst for ENRR due to the greater number of active sites, facile electron transfer, specificity and selectivity. The MPc taken for this study are NiPc, CoPc and CuPc which showed ammonia yield rate of 108, 85, 72 μ g h⁻¹ mg^{"-1}_{cat} and Faradic efficiency of 28, 25, 39% at –0.3, –0.3 and –0.4 V vs RHE respectively using 0.1 *M*HCl as an electrolyte.

Effects of antibiotics on biosorption of Cu²⁺ by Cu²⁺ resistant Saccharomy cescerevisiae

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This study reports the effect of antibiotics on 350 g/L resistant Cu^{2+} resistant strains of *S. cerevisiae* AB92. The strain was isolated from Baker's yeast, and it was made copper resistant gradually from low concentration to high concentration in laboratory conditions (tolerance study). So that it can tolerate and grow in the presence of copper and metabolize copper ions (characterization study has been done), antibiotics, when added in the fermentation medium of fungus in high concentration, can inhibit the growing fungus. The solution of each antibiotic was prepared separately. Results found that all tested antibiotics Streptomycin sulphate and Chloramphenicol exhibit maximum negative effect on cell growth of *S. cerevisiae* A92 and consequently biosorption of Cu^{2+} .

On the other hand, tetracycline-HCI, the potassium salt of penicillin, is found to have a bit inhibitory effect on cell growth and biosorption of Cu^{2+} by *S. cerevisiae* A92 at a higher concentration when added to the biosorption medium at an initial hour. Though Clotrimazole is a fungal antibiotic, it does not exhibit any drastic decline in cell growth or biosorption. At higher concentrations, it shows little negative effect on cell growth and biosorption of Cu^{2+} as well.

The effect of some different complex nutrients on bio-ethanol production from water hyacinth by ethanol and temperature resistant strain *Saccharomyces cerevisiae* AB₈₁₀

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The role of different complex nutrients on the production of bio-ethanol by the ethanol and temperature resistant strain Saccharomyces cerevisiae AB₈₁₀ to the selection of effective and suitable fermentation medium. Microorganisms have required specific nutrients for growth and metabolic activities. The type of organism as well as the nature of basal medium requirements of complex nutrient varies. To overcome the limitation of low productivity of ethanol, some conditions are to be established to the multiplication and successive function of the organism. During the bio-ethanol production, 25% (w/v) glucose and 0.3% (w/v) NaNO₃ served as the best carbon and nitrogen sources respectively. The optimum concentration of macro elements KH₂PO₄, and MgSO₄.7H₂O in fermentation is 0.10% and 0.05% repectively and trace elements ZnSO₄.7H₂O, Fe₂(SO₄)₃.H₂O, MnSO₄.7H₂O in fermentation 20 µg/ml, 15 µg/ml, 10 µg/ml respectively gives 12.2% (v/v) bioethanol production. Complex nutrient has contents amino acids, vitamins, minerals and carbon-nitrogen source, which is easily prepared or by-product some natural resource so it is low-cost nutrients than other chemical nutrients. In this study, it has been found that in addition to the above chemical elements, complex nutrient to the fermentation medium increases bioethanol production (13.2%) by Saccharomyces cerevisiae AB₈₁₀.

Systematic approach for development of ultrasound-assisted adsorption process for wastewater treatment

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Recently, water resources are in serious danger of being overused. In particular, water contamination has significant environmental consequences. The processing of huge quantities of wastewater has put a lot of pressure on humanity, in addition to the scarcity of water supplies due to drought and misuse. Different kinds of water contaminants exist. Among these contaminants, because of their high toxicity, the dyes are extremely harmful. The contamination of water sources by dyes as a result of their negative environmental consequences and human health is one of the most significant environmental concerns related to water pollution worldwide. Long residence times, high operation costs and energy consumption, and low efficiency are the main drawbacks of this traditional wastewater treatment technology. Coagulation, precipitation, sedimentation, filtration, solvent extraction, ion exchange, adsorption, electrodialysis, and membrane separation are some of the water pollution treatment technologies. Adsorption, on the other hand, is preferred in terms of convenience, ease of use, and design simplicity. In terms of efficiency, feasibility, spontaneity, and randomization, ultrasound-assisted adsorption is far superior. In this method, the best mode and adsorbent are chosen based on their simplicity, nontoxic and low-cost adsorbents, low treatment costs, and mild conditions. Because of its high operational and capital expenses, the need for regeneration and the decline in activity after regeneration, activated carbon is no longer the most extensively employed adsorbent. The demand for new adsorbents for the decolorization of aqueous solutions is increasing. Furthermore, it has been reviewed that combining ultrasonication and adsorption techniques can boost removal efficiency.
Applied Chemistry Lecture-20

Effect of epoxied vegetable oil (EVO) for flow assurance of waxy crude oil

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In low temperature condition, wax deposition from crude oil caused blockage in pipeline due to increase the viscosity of the fluid which is considered as a serious challenge for petroleum industry. Among different wax deposition mitigation techniques, chemical additives more specifically pour point depressants (PPDs) are widely applicable to solve this problem. The pour point and viscosity of the crude oil from Cambay basin were studied. The compositions with 1 and 2 wt% of EVO demonstrate better efficiency as PPD for crude oil than ethyl vinyl acetate copolymer (EVAc) at the dosage of PPD of 200, 500 and 1000 ppm. The presence of additional nonpolar and polar groups in the EVA copolymer was better to form EVAc/EVO composition. This part of the composition is similar to the wax crystals which can co-crystallize with wax crystal growth.

Study the effect of electrolytes and organic solvents in the synthesis of silica nanoparticles

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The impact of nanotechnology in human life plays an important role from 20th century. The size, structure, surface area, biocompatibility, vulnerability towards functionalization increase its acceptability in the field of health care, medicine, agriculture, technology etc. The global nano silica market was estimated 3348 kilo tons in 2015 and it is predicted the global market of nano silica will reach USD 5140.2 million by 2025. Herein, we describe a greener approach for the synthesis of silica nanoparticles. Specially, we are interested to understand the effect of various composition of organic solvents along with and without electrolytes in the modified Stobber method approach of silica nanoparticle synthesis. Tetraethylorthosilicate (TEOS) was used as precursor, NaOH as base and different concentration of ethanol, methanol and isopropanol starting from 20% to 60% were used as solvent. The mechanism of silica nanoparticle synthesis consists of mainly two steps: one is hydrolysis of TEOS and other one is condensation of silicic acid. Monitoring the concentration change in unreacted TEOS and soluble silica using molybdate assay in every reaction condition, a significant correlation have been drawn between the particle growth and their size. Use of electrolyte has a remarkable effect on growth and in final particle size specially using lower concentration of organic solvents. Sizes of particles was measured using Dynamic Light Scattering (DLS). Finally, a conclusion was drawn that using an electrolyte could be cost-effective while synthesizing higher sized nanoparticle at lower concentration of organic solvent.

Applied Chemistry Lecture-22

Applicability of bio additive towards petroleum industry

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In petroleum industry, of the many problem, wax deposition is very serious. Recent studies have focused on bio additive to solve the problem instead of conventional polymer as bio polymers are biodegradable, environmental-friendly and cost-effective. Different types of bio additives commonly known as wax dispersant, pour point depressants, wax crystal modifier are widely used to improve the flow properties of crude oil by reducing rheological properties like viscosity, yield stress etc. of crude oil. These bio additives are consisting of long aliphatic chain and polar moieties. The alkyl chain crystallizes with the paraffin waxes while the polar part prevents the extensive growth of wax crystal providing steric hindrance. The flowability of crude oil is increased by solubilizing the wax crystal. Natural resources like Vegetable oil, Amla, Shikakai, Ritha, Mahua are gained more interest to synthesize bio polymer. A natural polymer was prepared from olive oil and ethanol. The obtained product olive oil Ethyl ester (OE) was then modified with a bio based nano crystal (BC) and applied as PPD (OE-BC) to reduce the pour point of crude oil.

Applied Chemistry Lecture-23

Scale-up design methodology of the adsorption process

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Discharge of toxic heavy metals into our nature causes severe harm. Different plant operation generates heavy metal-bearing wastes, and discharging these wastes causes various damages to the living beings. Among the harmful elements, heavy metals played a major role as a pollutant because of their high toxicity and high persistence. Adsorption is an economical and efficient technique used for heavy metal removal. Various natural bioadsorbents, agricultural wastes, agricultural by-products, bio-polymers are available at low cost, which has good adsorptive capacity. Design of adsorption column using suitable adsorbents for industrial-scale minimizes the operating cost for wastewater treatment, which is beneficial for developing countries small and medium scale industries. The batch study and continuous column study are essential for the scale-up design for industrial purposes. Experiments were carried out to estimate the sorption capacity of various adsorbents and the effects of various operating parameters such as pH, column bed depth, influent flow rate, and influent metal ion concentration on the adsorption process. Different kinetic models were applied to the experimental result to investigate the process break through curve and best model, which will be further used for scale-up designing. In this study, a novel methodology of scale-up design for continuous operation is proposed. The results suggested that selected adsorbents could be used further for industrial wastewater treatment.

General Section

For Class-V to Postgraduate (PG) students

[1 - 29]

Fiber Reinforced Polymer (FRP)

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Fibre-reinforced polymer (FRP), also Fibre-reinforced plastic, is a composite material made of a polymer matrix reinforced with fibres. The fibres are usually glass, carbon, or aramid, although other fibres such as paper or wood or asbestos have been sometimes used. The polymer is usually an epoxy, vinylester or polyester thermosetting plastic, and phenol formaldehyde resins are still in use. FRPs are commonly used in the aerospace, automotive, marine, and construction industries.

Composite materials are engineered or naturally occurring materials made from two or more constituent materials with significantly different physical or chemical properties which remain separate and distinct within the finished structure. Most composites have strong, stiff fibres in a matrix which is weaker and less stiff. The objective is usually to make a component which is strong and stiff, often with a low density. Commercial material commonly has glass or carbon fibres in matrices based on thermosetting polymers, such as epoxy or polyester resins. Sometimes, thermoplastic polymers may be preferred, since they are moldable after initial production. There are further classes of composite in which the matrix is a metal or a ceramic. For the most part, these are still in a developmental stage, with problems of high manufacturing costs yet to be overcome. Furthermore, in these composites the reasons for adding the fibres (or, in some cases, particles) are often rather complex; for example, improvements may be sought in creep, wear, fracture toughness, thermal stability.

Fibre reinforced polymer (FRP) are composites used in almost every type of advanced engineering structure, with their usage ranging from aircraft, helicopters and spacecraft through to boats, ships and offshore platforms and to automobiles, sports goods, chemical processing equipment and civil infrastructure such as bridges and buildings. The usage of FRP composites continues to grow at an impressive rate as these materials are used more in their existing markets and become established in relatively new markets such as biomedical devices and civil structures. A key factor driving the increased applications of composites over the recent years is the development of new advanced forms of FRP materials. This includes developments in high performance resin systems and new styles of reinforcement, such as carbon nanotubes and nanoparticles. This book provides an up-to-date account of the fabrication, mechanical properties, delamination resistance, impact tolerance and applications

of 3D FRP composites.

The fibre reinforced polymer composites (FRPs) are increasingly being considered as an enhancement to and/or substitute for infrastructure components or systems that are constructed of traditional civil engineering materials, namely concrete and steel. FRP composites are lightweight, no-corrosive, exhibit high specific strength and specific stiffness, are easily constructed, and can be tailored to satisfy performance requirements. Due to these advantageous characteristics, FRP composites have been included in new construction and rehabilitation of structures through its use as reinforcement in concrete, bridge decks, modular structures, formwork, and external reinforcement for strengthening and seismic upgrade.

The applicability of Fiber Reinforced Polymer (FRP) reinforcements to concrete structures as a substitute for steel bars or prestressing tendons has been actively studied in numerous research laboratories and professional organizations around the world. FRP reinforcements offer a number of advantages such as corrosion resistance, non-magnetic properties, high tensile strength, lightweight and ease of handling. However, they generally have a linear elastic response in tension up to failure (described as a brittle failure) and a relatively poor transverse or shear resistance.

They also have poor resistance to fire and when exposed to high temperatures. They loose significant strength upon bending, and they are sensitive to stress-rupture effects. Moreover, their cost, whether considered per unit weight or on the basis of force carrying capacity, is high in comparison to conventional steel reinforcing bars or prestressing tendons. From a structural engineering viewpoint, the most serious problems with FRP reinforcements are the lack of plastic behavior and the very low shear strength in the transverse direction. Such characteristics may lead to premature tendon rupture, particularly when combined effects are present, such as at shear-cracking planes in reinforced concrete beams where dowel action exists. The dowel action reduces residual tensile and shear resistance in the tendon. Solutions and limitations of use have been offered and continuous improvements are expected in the future. The unit cost of FRP reinforcements is expected to decrease significantly with increased market share and demand. However, even today, there are applications where FRP reinforcements are cost-effective and justifiable. They also have poor resistance to fire and when exposed to high temperatures. They loose significant strength upon bending, and they are sensitive to stress-rupture effects. Moreover, their cost, whether considered per unit weight or on the basis of force carrying capacity, is high in comparison to conventional steel reinforcing bars or prestressing tendons. From a structural engineering viewpoint, the most serious problems with FRP reinforcements are the lack of plastic behavior and the very low shear strength in the transverse direction. Such characteristics may lead to

premature tendon rupture, particularly when combined effects are present, such as at shearcracking planes in reinforced concrete beams where dowel action exists. The dowel action reduces residual tensile and shear resistance in the tendon. Solutions and limitations of use have been offered and continuous improvements are expected in the future. The unit cost of FRP reinforcements is expected to decrease significantly with increased market share and demand. However, even today, there are applications where FRP reinforcements are costeffective and justifiable.

Without Water, Everything Withers

Ananya Prasad

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Water is the basic necessity of every living organism but water crisis is one of the major problems in India. Water is the central point of our lives but unfortunately is not our priority concern. You never know the worth of **water** until the well runs dry. In many states the wells have already dried up although the citizens aren't concerned. The crisis has become so severe that in many places/states the groundwater level has depleted. Many villages don't get water to drink everyday they need to save some amount of water for the consecutive days. We need to think and work upon this topic if we are worried for the future generations to come.

In my presentation/poster I will inculcate the following points about conservation of water:-

- How can we save water?
- Why is water wasted?
- How do people waste water?
- Why don't people care about water?
- How can we cajole people to save water?
- What if water isn't sufficient for the generations to come?

I will try to put pictures, drawing, self-made model's description, poem, slogans, paragraphs in my poster.

Impact of Immune Boosters in Covid-19

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Covid-19 or Coronavirus was declared as a global pandemic by the World Health Organization. And while the countries are grappling with imminent dangers that this virus poses to humanity, increase in immunity as become a necessary to preventing disease, rather than treating it. Food plays a key aspect in determining our overall health and immunity. People tend to have less robust immune responses as they age, and the elderly are more prone to infection and have lower protection rates from vaccines. The development of the immune response through neonatal, infant and adult life, including pregnancy, ending with the decline in old age is different. Immune boosters such as Vit C, Vit D, nutrients and other powerful antioxidants helps in cells anti-viral mechanism to fight against the virus in a better way. Protein, zinc, omega 3 fatty acids, vitamin D, antioxidant rich foods and prebiotic and probiotic containing foods are very necessary to keep our immune system healthy during Covid-19 pandemic. The young (non-pregnant) adult organism seems to be perfectly equipped for this challenge. COVID-19 patients have significantly low counts of a cell type that plays a crucial role in immune response, with lower numbers of these cells indicating more severe disease, according to a study whose findings may lead to the development of new therapeutics against the disease. Immune boosters if taken in a sufficient quantity required for a healthy body helps the cells anti-virus mechanism mainly because of its anti-oxidant and antiinflammatory properties.

Everyone should focus on "PREVENTION" rather than "CURE".

Corona virus: Prevention and possible remedial measures

Sreyasi Talukdar

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Novel coronaviruses (CoVs), responsible for severe respiratory syndromes and post covid illness for mostly comorbid cases, have raised concerns about global public health emergencies over the past two years. To limit the infections, we need to understand the process of virus spread to take action against this transmission. Chemists have produced antiviral materials and coatings which can be used for surfaces and personal protective equipment (PPE) to reduce transmission. There are air filters, UVC light, etc. and other filtration techniques are being used to destroy viruses in the air. Thus some processes can be discussed which are being applied in the prevention of coronavirus and are on the way to be discovered for the same purposes.

We were born to help the world, not to destroy it

Janaki Nadan Dey Class-V St. Michael's School, Bankura-722 101, West Bengal, India

An environment is a nature that nurtures our life on the earth. Everything which we feel, breathe, and eat in our life comes from the environment. Like land, plants, water, air, sunlight, forests, food, rivers, and other natural things come within the environment. The existence of our healthy life depends on the environment which maintains nature's balance. It is important to save our environment and maintain nature's balance for the existence of life.

An environment should be safe and clean, without it we cannot imagine the existence of our life in the future. Many health diseases and disorders increasing due to water and air pollution. Water pollution occurs due to the release of unrefined industry wastes and other unsafe elements into the water. The air is polluted due to the uncontrolled discharge of harmful smoke from vehicles and industries. Soil and noise pollution also impacts our environment. Environmental pollution is impacting negatively on many factors of our daily life. People should take part in afforestation to make a healthy environment. We must take a strong initiative to protect the environment. It is important that everyone should put a little effort to bring a positive change in the destruction of the environment. We should take an initiative to make our environment safe and pollution-free.

We can protect the environment in different ways and everybody should come forward and take part in the environmental safety campaign. World Environment Day is an environment safety event celebrated on 5th June every year across the world. So, it is the responsibility of every human being to save the environment. So that the next generation may enjoy the gifts of nature.

Factors that Threaten Human Life through our surroundings

Sarvadeb Mandal

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The environment plays a crucial role in the proper development of all the living organisms on this beautiful Earth. The conditions and nature of pollutants in our surroundings play a vital role in determining the quality of life. The essential things for our daily life as food, water, shelter, education and hospital depend on the environment around us. There are several harmful effects of human activities like air to water pollution, over-population, waste disposal, climate change, global warming, and the greenhouse effect, are the big reason that poses a serious threat to human lives. Therefore, we must spread environmental awareness in our society and we will maintain in our routine life, which is our responsibility. It is necessary to save and protect our environment towards a greener and more sustainable future.

Automatic tank without sensor

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This is a very simple mechanism which we can use with any kind of water tank. The main feature of this tank is that it prevents from waste a single drop of water and the electricity. As this mechanism will be fit with the top of the tank it simply do that when the tank gets filled it automatically stops the pump, when the pump will not run after the filling of the tank it saves both the electricity as well as water.

The main reason for selecting this idea because it is very affordable, it is a effective, it can work anywhere at any condition, and also it have no maintenance charges, it is also customizable and it also don't have any installation charges.

It is a project which is very effective in the arid and low water regions. It is so simple that it can use by any people.

It has a simple parts on a box which have two electricity conducting metal top of the tank and placing at 180° to each other, it also have a safety case over it, which have one more long stick of metal which can connect the both. It also has a ball like object inside the tank which can create a high buyout force. And the two electricity conducting metals on the top of the tank will be connected with the terminal with the water pump like a switch. It works with the simple physics formula of the buoyant force. As the water gets fill the tank slowly, the ball which present inside the tank also raise with the water and the electricity conducting metal also raise and break the circuit as a result the pump stops working, and the water also not overflow from the tank.

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Our environment, our life

Pritilata Patra Class-V Govt. Model School, Nayagram, Paschim Medinipur, West Bengal, India



Corona viruses: Prevention and possible remedial measures

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Coronaviruses are a family of viruses that can cause respiratory illness in humans. They get their name, CORONA, from the many crown like spikes on the surface of the viruses. Coronaviruses, like the new COVID-19 outbreak that began in China, cause mild to severe respiratory illness including death. COVID-19 has since spread worldwide. A person can be at risk if they have any of the following symptoms: fever and symptoms of lower respiratory illness such as coughing or difficulty in breathing.

So prevention is better than cure.

- 1. Avoid close contact with those who are sick.
- 2. Feeling sick? Stay at home.
- 3. Cover your mouth when you cough or sneeze.
- 4. Quarantine those who are sick.
- 5. Regularly clean doorknobs handles and tables with soap and water.
- 6. Use a sanitizer with at least 60 percentage alcohols.
- 7. Don't share face masks.
- 8. Use soap and water to wash your hands for 20 seconds.

Possible remedial measures are like -

- 1. Clean your hands often
- 2. Cough or sneeze in your bent elbow, not your hands!
- 3. Avoid touching your eyes, nose and mouth.
- 4. Avoid close contact with someone who is sick.
- 5. Limit social gatherings.

Clean and disinfect frequently touched objects and surfaces.

Corona virus: Prevention and possible remedial measures

Zainab Khatun

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We have witnessed loss, suffer and resilience all brought up by the Covid-19 pandemic. We spent past year finding solutions to get rid of this virus. A nationwide lockdown was imposed, the think tank formulated policies for the poverty stricken population to get the financial support and resources while lockdown was imposed, doctors and healthcare staff devoted their time 24×7 for treatment and care of patients and scientists all over the world tried to find the permanent solution to the problem by developing a vaccine and all of us became accustomed to this 'new normal'.

The virus still is there. We still are no way near to the 'old normal', then where did we go wrong? And more importantly will the pandemic ever end and how? Is it at all stoppable?

Well, if we look at our past the truth of the matter is that pandemics always end. And to date vaccines have never played a significant role in ending them. (That doesn't mean vaccines aren't playing a critical role this time. Far fewer people will die from Covid-19 because of them, is what scientists believe).

There were no flu vaccines in 1918, when the world didn't yet know that the great influenza was caused by a virus, H1N1. In 1957, when the H2N2 pandemic swept the world, flu vaccine was mainly a tool of the military. In the pandemic of 1968, which brought us H3N2, the United States produced nearly 22 million doses of vaccine, but by the time it was ready the worst of the pandemic had passed, and demand subsided. again in 2009, when the world finally had the capacity to make hundreds of millions of doses of H1N1 vaccine; some countries canceled large portions of their orders because they ended up not needing them.

How did those pandemics end? The viruses didn't go away; a descendant of the Spanish flu virus, the modern H1N1, circulates to this day, as does H3N2. Humans didn't develop herd immunity to them, either, the phenomenon by which a pathogen stops spreading because so many people are protected against it, because they've already been infected or vaccinated.

Instead, our immune systems learned enough about them to fend off the deadliest manifestations of infection, at least most of the time. Humans and viruses reached an immunological detente. Instead of causing devastating illness, over time the viruses came to trigger small surges of milder illness.

Pandemic flu became seasonal flu. The viruses became endemic.

Experience from the last four pandemics suggests that viruses morph from pandemic pathogens to endemic sources of disease within a year and a half or two of emerging. But all of those pandemics were influenza pandemics. A different pathogen could mean we'll see a different pattern. But what we are assured of is that the pandemic will end.

So can prevention on an individual level help us achieve it faster somehow? And what are the possible remedial measures, and if at all there is any?

I'll be discussing what preventive measures actually helps in slowing down the development of COVID-19 and reduce the risk of overwhelming the health care system.



This chart illustrates how protective measures such as limiting travel, avoiding crowds, social distancing, and thorough and frequent handwashing can slow down the development of new COVID-19 cases and reduce the risk of overwhelming the health care system.

Source: https://www.health.harvard.edu/diseases-and-conditions/preventing-the-spreadof-the-coronavirus

Since the most popular remedial measure for COVID is vaccines, I'll talk about the credibility of vaccines. I'd try to answer the question "can COVID vaccines stop transmission?"

We were born in the earth to protect the earth, not to pollute it

Devdutta Dey Class-V St. Lawrence High School, Kolkata-700 019, India

Environment can be defined as a sum total of all the living and non-living elements and their effects that influence human life. Environment on earth is essential to every aspect of human life. It includes sunlight, atmosphere, land, water, plants, animals, sea life, minerals, different species and everything that occurs naturally on earth. The environment in which we live providing constant natural services to humans and all other species since the beginning of life on earth. Though it is not a new phenomenon, yet it remains the world's greatest problem.

To live in safely on Earth we must protect our environment. But in today's world, environment is getting polluted more and more. Out of many pollutions, air pollution poses the greatest environmental risk today. Major sources of air pollution are forest fire, smoke from industries and from vehicles, burning of fossil fuels, deforestation, open burning of garbage waste, etc. Other pollution that are damaging our environment in many ways is water pollution. For example untreated industrial wastes, oil spills, dumping wastes in water, Sewage and wastewater treatment, radioactive wastes, pesticides and chemical fertilizers, etc. Water pollution is the leading worldwide cause of death and disease. Moreover, there are soil pollution and noise pollution that are damaging our environment.

Because of this pollution our environment is getting affected severely. Some of the major effects are global warming, ozone depletion, increase of sea water level, hazards to wildlife, disruption of ecosystem, threats to marine life, various water borne diseases, Loss of soil nutrients, hearing loss, sleeping disorder etc.

So, we must protect our environment by any means. We can protect our environment by using battery-powered vehicles, disposing treated industrial wastes, stopping use of chemicals that are harmful, stopping deforestation, planting more trees, etc. We should also participate in safety campaigns and come forward to protect our environment. We should celebrate World Environment Day, which is celebrated on 5th June every year, in a greater way.

A study on mutation of Coronavirus

Debolina Dey Undergraduate (UG) Victoria Institution College, Kolkata-700 009, India

India was facing one of the worst cases of 2nd wave Covid-19 virus.

Even though several vaccines were available in our country. We were still facing severe cases from the virus because of several factors including public negligence towards the consequences and the future danger of the virus.

New strains of the virus have been found in different areas of the world. Scientist are still discovering and predicting future strains of this virus.

Although present vaccines are pretty efficient towards the present strains, but if this mutation keeps happening we may reach a point where the present vaccines will be less efficient and mayl cause great chaos and severe problems.

This is one of the reasons why it's necessary for people to know about the future consequences of the virus if we fail to break this vicious chain.

Everyone should take the vaccine and keep maintaining the rules and regulations implemented by the government for our own safety. This will help us break the chain of further unknown mutations of this virus. This will eliminate the virus or its effectiveness from the environment forever.

Our environment, our life

Anushka Dinda

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The surroundings and condition in which we live is known as our environment. All living things that live on this earth comes under the environment. Whether they live on land or water they are part of the environment. The environment also includes air, water, sunlight, plants, animals, etc.

Moreover, the earth is considered the only planet in the universe that supports life. The environment can be understood as a blanket that keeps life on the planet sage and sound.

We should care for our environment to survive in this planet or else one day will come when the planet will have only land and waterbodies.

Water crisis and conservation

Bitihotra Roymahapatra Class-IX Vivekanada Mission School, Haldia-721 631, West Bengal, India

Water scarcity or water crisis is the lack of fresh water resources to meet the standard requirement. Humanity is facing water crisis due to unequal distribution of fresh water, resulting in some very wet and some very dry geographic locations. And in addition to it, a sharp rise in global freshwater demand, driven by industry, has also contributed largely to the scant water supply. Water scarcity can also be caused by droughts, lack of rainfall, or pollution. The World Economic Forum in 2019 predicted potable water crisis as one of the largest global risks in terms of potential impact over the next decade. It is manifested by partial or no satisfaction of expressed demand, economic competition for water quantity or quality, disputes between users, irreversible depletion of groundwater, and negative impacts on the environment. Two-thirds of the global population (4 billion people) live under conditions of severe water scarcity at least 1 month of the year. Half a billion people in the world face severe water scarcity all year round. Half of the world's largest cities experience water scarcity.

The essence of global water scarcity is the geographic and temporal mismatch between fresh water demand and availability. The increasing world population, improving living standards, changing consumption patterns, and expansion of irrigated agriculture are the main driving forces for the rising global demand for water. Climate change, such as altered weather-patterns (including droughts or floods), deforestation, increased pollution, green house gases, and wasteful use of water can cause insufficient supply. At the global level, on an annual basis enough freshwater is available to meet such demand, but spatial and temporal variations of water demand and availability are large. This leads to (physical) water scarcity in several parts of the world during specific times of the year. Scarcity varies over time as a result of natural hydrological variability, but varies even more so as a function of prevailing economic policy, planning and management approaches. Scarcity can be expected to intensify with most forms of economic development, but, if correctly identified, many of its causes can be predicted, avoided or mitigated.

The International Resource Panel of the UN states that governments have tended to invest heavily in largely inefficient solutions: mega-projects like dams, canals, aqueducts, pipelines and water reservoirs, which are generally neither environmentally sustainable nor economically viable. The most cost-effective way of decoupling water use from economic growth, according to the scientific panel, is for governments to create holistic water management plans that

take into account the entire water cycle: from source to distribution, economic use, treatment, recycling, reuse and return to the environment.

Physical water scarcity is where there is not enough water to meet all demands, including that needed for ecosystems to function effectively. Arid regions frequently suffer from physical water scarcity. It also occurs where water seems abundant but where resources are overcommitted, such as when there is overdevelopment of hydraulic infrastructure for irrigation. Symptoms of physical water scarcity include environmental degradation and declining groundwater. Water stress harms living things because every organism needs water to live.

Physical water scarcity results from inadequate natural water resources to supply a region's demand, and economic water scarcity results from poor management of the sufficient available water resources. According to the United Nations Development Programme, the latter is found more often to be the cause of countries or regions experiencing water scarcity, as most countries or regions have enough water to meet household, industrial, agricultural, and environmental needs, but lack the means to provide it in an accessible manner. Around one-fifth of the world's population currently live in regions affected by physical water scarcity, where there are inadequate water resources to meet a country's or region's demand, including the water needed to fulfil the demand of ecosystems to function effectively. Arid regions frequently suffer from physical water scarcity. It also occurs where water seems abundant but where resources are over-committed, such as when there is over-development of hydraulic infrastructure for irrigation. Symptoms of physical water scarcity include environmental degradation and declining groundwater as well as other forms of exploitation or overuse.

There are many ways to conserve water industrially as well as in domestic use. Like :

- Rain water harvesting to be done
- Low flush urinals or vacuum chambered toilets to be used
- Water treatment plants need to be set up at a large scale to reuse the waste water
- Hand and object sensing taps to be installed for zero wastage of water
- Low wastage irrigation system like overhead irrigation system
- Low wastage car washers to be used in washing centres
- Stop draining harmful wastes to fresh water sources like rivers
- Serious concern to be given in waste management department
- Limiting the use of water by houses in urban areas

This are the easiest ways we can use to save water for our future from today. Life is not possible without water, so we have to be concerned on the wastage of water and also how we can conserve it from now onwards. Save water to save lives. With this I end my speech here.

Periodic table revisited – Necessity of rules

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A new theoretical concept have been constructed here in this communication, which can be used to calculate the group, period and also atomic number of any element naively by using simple algebraic equations, based on three completely new rules, named as Noble Gas rules for periodic table. The real wonder of this new formulation lies in the fact that these rules help in calculating the group of any given element and finding out the atomic number of any element very easily. The strong part of this new theoretical concept we will not use electronic configuration method for calculating the groups and periods and it can be applicable anywhere in the periodic table. This concept can be used to find out the atomic number and position of any element in any period of a particular group, if the atomic number of one element is given. Our current theoretical concept is absolutely novel in the way that it is trying to develop new kind of orientation in the minds of Chemistry people dealing with Periodic table – irrespective of students, teachers, scientists.

Ru-based anti-cancer drug: An alternative approach

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Cancer accounts for three of the top ten leading causes of death for people all over the world, and is the primary cause of approximately 12.5% of all deaths world-wide per year, according to the International Agency for Research on Cancer (IARC). In India, it is estimated that 14.5 lakh people are living with the disease, with over 7 lakh new cases being registered every year and 5,56,400 deaths which are said to be cancer related. An estimated 71% of all cancer related deaths are occurring in the age group between 30 to 69 years. Currently, chemotherapy is the most used treatment all over the world against cancer. But recent study shows that it has some side effects such as multidrug resistance, relapse, and off-target cytotoxicity, etc. and leave an ever-increasing need for exploring alternative modes of treatment. Rosenberg's discovery was certainly the most outstanding since it led to the marketing of cisplatin, the first anticancer metal complex and still one of the three most used drugs in oncology. Not only cisplatin, there are so many others anticancer metal complexes like (platinum based) Carboplatin, Oxaliplatin, Heptaplatin, (Ruthenium based) NAMI-A, KP1019, NKP-1339, (copper based) Casiopeinas etc. in market or in clinical trial. Ruthenium complexes have attracted increasing interest in the last two decades as a new generation of metallodrugs. Ruthenium compounds have shown selective bioactivity and the ability to overcome the resistance that platinum-based therapeutics face, making them effective oncotherapeutic competitors in rational drug invention approaches. The development of antineoplastic ruthenium therapeutics is of particular interest because ruthenium containing complexes NAMI-A, KP1019, and KP1339 entered clinical trials and DW1/2 is in preclinical levels. The very robust, conformationally rigid organometallic Ru(II) compound DW1/2 is a protein kinase inhibitor and presents new Ru(II) compound designs as anticancer agents. Over the recent years, numerous strategies have been used to encapsulate Ru(II) derived compounds in a nanomaterial system, improving their targeting and delivery into neoplastic cells. A new photodynamic therapy based Ru(II) therapeutic, TLD-1433, has also entered clinical trials. Ru(II)-based compounds can also be photosensitizers for photodynamic therapy, which has proven to be an effective new, alternative, and noninvasive oncotherapy modality.

Our environment, our life

Ooisheerup Adak Class-VI Dolna Day School Kolkata

Environment plays a significant role in healthy living so that life could sustain on planet earth. Without the surrounding there cannot be existence of any life in the planet earth. It gives food, shelter, air, and fulfills all the human needs. Nowadays, Scientist have found that we, the human are causing harm to our mother Earth. We should plant more and more trees, use of CNG vehicles to save our environment and life.



Sustainable development: Future agroindustry agrohomeopathy

K. Srikant

Class-VIII Sri Chaitanya Techno School Kolkata

Homeopathy is known to be aA Nano Technology based healing technique which has now been used to increase crop production. Kaviraj is a pioneer in the field and when this is popularized among the farmers and more of agrohomeopathy is used there will be a sustainable agriculture in future. The poster will deal with the works and knowledge of agrohomeopathy that will help us in practicing in home garden.

Sustainable agriculture solutions

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Agriculture is the world's largest industry. Intensive agriculture, as it has been practiced since the 1960s, has very high yields, but depletes the soil and pollutes the environment such as greenhouse gas emissions, biodiversity loss, ocean acidification, etc. The limits of Natural Resources and the pollution of air, water and soil has introduced awareness and pushed the society for the use of sustainable farming. Green agriculture is the application of the sustainable development principles to agriculture which ensures the production of food, wood and fibers and at the same time it also respects the ecological, economic and social limits that ensure the durability of this production. For instance, sustainable farming minimises the use of pesticides that can harm the health of farmers and consumers.

Sustainable energy – The need of the hour

Manan Tripathi

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Sustainable energy is a form of energy that meets our today's demand of energy without putting them in danger of getting expired or depleted and can be used over and over again. Sustainable energy should be widely encouraged as it does not cause any harm to the environment and is available widely free of cost. All renewable energy sources like solar, wind, geothermal, hydropower, and ocean energy are sustainable as they are stable and available in plenty. This energy is replenishable and helps us to reduce greenhouse gas emissions and causes no damage to the environment.

Our environment, our life

V. Sharnitha

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All the physical surroundings on earth are called the environment. Environment plays a vital role in healthy living and the existence of life on the planet is called earth.

The environment includes everything living and non living things. The peoples, animals and plants on planet and all the living things relay on the non living parts to survive in the environment. The life happens are called the biosphere. It is very important all of us to save and protect our environment. Environment means any things that surround us; it can be living biotic or non-living abiotic things. It includes physical, chemical and other naturals. We are all dependent on the environment for food, air, water and other needs. People should conserve the environment by avoiding ecology damages. We should grow more plants and environment friendly activities. We must avoid global warming by safe guard the climate condition on earth. Preserve of the earth and ecology by creating more awareness on the topic among peoples and should strictly follow the same.

It is also cover all living species, climate, weather and natural resources. Environment is responsible for nourishing the life exists on the earth. Natural disasters are temporary in nature but can be safeguard the nature.

Life is thriving on good environment, where living species needs basic things like air, water and vegetations are available on the earth, where environment is highly protected and life without environment is unimaginable. The quality of life is directly associates with quality of Environment. If environment degrade, it affects life on several ways. A chemical brings new environmental problems and harmful unexpected side effects. Natural eco-friendly chemical products are need of the hour. Various heavy industries are prime source for environmental pollution i.e. leather industry, petroleum industry and textile industry etc. Humans are affected by various ailments that are industrial effluents, gases i.e. carbon monoxide and nitric oxide from automobiles, pollutants, dyes, insecticides and pesticides. We humans are must take care of environment for self sustain of life on earth. Life is precious in nature, so we must respect and adore the joys movement of life.

More exploitation of natural resources brings environment degrade to the life. Life is protected by safe environment.

"Save Life, Save tree, Save nature, Save resources, Safe life and environment".

Corona Virus: Prevention and possible remedial measures

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Corona viruses are a group of related RNA viruses that cause diseases in mammals and birds. In humans and birds, they cause respiratory tract infections that can range from mild to lethal. Mild illnesses in humans include some cases of the common cold (which is also caused by other viruses, predominantly rhinoviruses), while more lethal varieties can cause SARS, MERS, and COVID-19. In cows and pigs they cause diarrhea, while in mice they cause hepatitis and encephalomyelitis.

Conserve water save life

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In our daily lives, water is the most important resource. Every day, we should drink 2 to 3 litres of water. Water covers around 71 percent of the Earth's surface. However, just 3% of it is drinkable. At least 2 billion people worldwide consume water that has been polluted with various contaminants. According to the World Health Organization, half of the world's population will live in water-stressed areas by 2025. There will be no water in 2040 if we do not preserve water. Nowadays, water is polluted by a variety of chemicals, resulting in pollution. Drinking water, rivers, lakes, and seas across the world are impacted by pollution.

Water pollution is defined as any alteration in the physical, chemical, or biological characteristics of water that has a negative impact on any living creature.

Thus, we need to conserve water for our safe future.

Water crisis, conservation and harvesting

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Water is essential for survival and for development of civilisation. Living cells are composed of more than 90% water; the interactions between water and the other constituents of cells are of central importance in biological chemistry. About 80% illnesses are associated with poor quality drinking water and rough sanitation. Ancient Indians knew harvesting of water 7000 years ago making wetlands. Wetlands are cradles of biological diversity and are among the world's most productive environments. Although 2/3 of the earth is filled with water but potable water is only <1%. In my talk I will focus on causes of water pollution, water harvesting and scientific use of water.

"Chemistry for Better Tomorrow" Our Environment, Our Life

Ojasvini Singh

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- I am presenting my poster.
- > The theme of my poster is 'Our Environment, Our Life'.
- > In my poster, I have drawn and painted **Our Mother Earth** and Her Environment.
- > The hands in the poster symbolize the protection and care to the Environment.
- > STAY AT HOME STAY SAFE during the COVID-19 pandemic.
- > We should not pollute our environment.
- > We must take care of our Environment today so that there will be a life tomorrow.


Future Agro Industry Edible Mushroom: The Future Agro Industry

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It is a chain process connecting agriculture and its products with different levels of industry where those products are processed in to different useful materials make them become more valuable in the modern society. This helps to upgrade the economy of people related to the total process and generating a demand in the market globally.

In the fast transforming modern and developing society one of such agriculture - industry based hybridized topic or material is mushroom. Mushrooms can grow very easily not only in open space but also in very small space even in a room of home and it requires limited infrastructural facility. Though there are different types of mushrooms, most of them are not edible or toxic but several contain high nutritional value having medicinal and therapeutic or healing effect which makes it precious and very useful and more demandable among the modern society. Edible mushrooms are processed in various forms in the small medium and large industries such as Mushrooms powders, Mushrooms soups, Tablets (medicines), Tea and Spices etc. which become more acceptable in the market.

Already mushrooms and its processed products has a large demand or popularity throughout the state and country also it has some global impacts. And if it becomes more popular the Economical and Industrial state can be upgraded. So these kinds of Industry connecting to the agricultures and its popularity, demand, market, modern socioeconomical impact have a huge scope to be upgraded in the future as Agro Industry.

Sustainable development: Future Agroindustry Future of Agriculture in a post-pandemic World

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Agriculture is on the frontlines of nearly all urgent global challenges, from hunger to climate change to rising inequality. Investment in agriculture has an important poverty-reduction effect especially amongst the poorest people. COVID-19 pushed 130 million more people into hunger by the end of 2020. Food production and agriculture matter: they provide livelihoods for more people in the world than any other sector. The pandemic is having a marked impact on both the production and consumption of agricultural produce. On the demand side, it is reducing food security, due to the loss of jobs and declines in wage income. The number of persons in the region living in extreme poverty, which correlates closely with hunger, is expected to increase. The emergency has lowered international prices for most staple products. On average, between January and April 2020, international food prices fell by 9.1%, compared to drops of 12.5% for minerals and 47.9% for energy.

To sustain the stability in development in May 2020, the Indian government announced a COVID-19 economic relief package called "Atmanirbhar Bharat (Self Reliant India)" totaling about USD \$270 billion. The main components among the package's are a set of changes to laws governing agriculture markets – in other words, the government has used the COVID-19 crisis as an opportunity to push through significant agricultural reforms that will have many medium- and long-term impacts.

Energy sustainability

Roheena Pal

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Sustainable development has three major components: (1) Economic growth, (2) Environmental Stewardship and (3) Social Inclusion. Energy sustainability is one part of it. Sustainable energy is about finding alternative renewable sources of energy – sources that renew themselves, rather than sources that can be depleted. It's called sustainable energy because it can sustain us for the long term. Sustainable energy includes all renewable energy sources, such as hydroelectricity, geothermal, wind, idal and solar energies. Solar energy is the best form of sustainable energy. Solar energy is radiant light and heat from the sun that is harnessed using a range of modern technologies such as solar heating, photovoltaics, solar thermal energy, solar architecture, molten salt power plants and artificial photosynthesis. Wind power is extracted from air flow using wind turbines or sails to produce mechanical or electrical power. Wind mills are used for mechanic power, wind pumps for water pumping and sails to propell ships. The energy which is obtained from the strong currents of water produced by the rise and fall of sea level due to tidal action is called tidal energy which can be captured and converted to electricity. The energy which is generated by utilising the heat of the earths interior is called geothermal energy. The geothermal heat pump represents an emerging technology marked with impressive market growth. Besides some non-conventional sources like biomass and hydrogen are suggested to be used frequently. In addition, energy efficiency and energy conservation are the new approaches towards energy sustainability. Energy is needed to support various activities of the civilized society. However, the actual amount of energy required depends on the efficiency with which it is used which in turn depends on the technology, the integration of energy systems and energy conservation practices. Apart from that we should follow some best practices like use of water-efficient fixtures. But sustainable technology is the pre-requisite of energy-sustainability, which is a monumental challenge indeed. With environmental issues like global warming, habitat destruction, and many other socio-environmental issues becoming more pressing, it is clear that we need to invest in more sustainable practices.

জল সঙ্কট এবং সংরক্ষণ

অরিত্রিকা দাস মহাপাত্র

ক্লাস-X, মোহনপুর উচ্চ বিদ্যালয় (H.S.)



অক্সিজেন এবং জল ছাড়া আমাদের এক মুহূর্তও বেঁচে থাকা সম্ভব নয়। কিন্তু দুঃখের বিষয় হল, বুদ্ধি এবং মেধার বলে আমরা চাঁদ পর্যন্ত পৌঁছে গিয়েছি ঠিকই। কিন্তু প্রতিনিয়ত অবুঝের মতো গাছ কেটে অক্সিজেনের ঘাটতির মাত্রা যেমন বাড়াচ্ছি, তেমনই অকারণ জলের অপচয় বাড়ার কারণে মাটির নিচে যে জলের মাত্রা ক্রমশঃ কমছে, তাও আমাদের গোচরে রয়েছে। তবু যে কেন জলের ঘাটতি মেটানোর কোনও প্রয়াস আমরা করছি না, সে বিষয়ে প্রশ্ন উঠতে বাধ্য। কারণ, পরিস্থিতি দিনে-দিনে ভয়ঙ্কর রূপ নিচ্ছে। একাধিক সমীক্ষার পরে একথা জলের (Water) মতো পরিষ্কার হয়ে গেছে যে এখন থেকেই যদি জলের খরচ বাঁচানোর নিকে নজর ফেরানো না হয়, তাহলে আগামী কয়েক বছরে মারাত্মক জলের ঘাটতি দেখা দেবে। তখন হাজার-হাজার টাকা খরচ করেও কিন্তু জলের চাহিদা মেটানো সম্ভব হবে না। তাই সাবধান হতে হবে এখন থেকেই। কীভাবে জলের অপচয় কম (How to Conserve Water) করবেন, তাই ভাবছেন নাকি? চিন্তা নেই বন্ধু।

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Note : *Mark indicates the senior author of the paper and [†]mark indicates the author who will be presenting the paper