The Celebration of the 161st Birth Anniversary of Acharya Prafulla Chandra Ray
&
International Seminar on Recent Advances in Chemistry and Material Science

(RACMS-2022)

[July 30-31 (Online) & August 2 - 3, 2022]

- ❖ Young Scientists' Conclave (YSC - 2022)
- ❖ Research Scholars' Competition (RSC - 2022)

Organized by

Indian Chemical Society, Kolkata

In Association with the
Bangladesh Chemical Society, Bangladesh
&
Department of Chemistry, Jadavpur University, Kolkata

Venue

The Ramakrishna Mission Institute of Culture, Golpark, Kolkata (August 02, 2022)
&
Dr. Triguna Sen Auditorium, Jadavpur University, Kolkata (August 03, 2022)

The Celebration of the 161st Birth Anniversary of Acharya Prafulla Chandra Ray

&

International Seminar on Recent Advances in Chemistry and Material Science

(RACMS-2022)

[July 30-31 (Online) & August 2 - 3, 2022]

- **Young Scientists' Conclave (YSC - 2022)**
- **Research Scholars' Competition (RSC - 2022)**

Organized by

Indian Chemical Society, Kolkata

In Association with the
Bangladesh Chemical Society, Bangladesh
&
Department of Chemistry, Jadavpur University, Kolkata

Venue

The Ramakrishna Mission Institute of Culture, Golpark, Kolkata (August 02, 2022)
&
Dr. Triguna Sen Auditorium, Jadavpur University, Kolkata (August 03, 2022)

International Seminar on
Recent Advances in Chemistry and Material Science (RACMS-2022),
Young Scientists' Conclave (YSC-2022) & Research Scholars' Competition (RSC-2022)

The 161st Birth Anniversary Celebration of Acharya Prafulla Chandra Ray

Advisory Committee (2022)

Professor G. D. Yadav	President, Indian Chemical Society
Swami Suparnanandaji Maharaj	Secretary, RKM Institute of Culture, Golpark
Professor R. D. Kaushik	Vice-President, Indian Chemical Society
Professor Shubhangi Soman	Vice-President, Indian Chemical Society
Professor A. C. Bhasikuttan	Honorary Editor
Professor Samaresh Bhattacharya	Honorary Editor
Professor Chhanda Mukhopadhyay	Honorary Editor
Professor Suresh C. Ameta	Advisor, Indian Chemical Society
Professor Dulal C. Mukherjee	Advisor, Indian Chemical Society
Professor D. Banerjea	Advisor, Indian Chemical Society
Professor Jai P. Mittal	Advisor, Indian Chemical Society
Professor K. B. Pandeya	Advisor, Indian Chemical Society
Professor Ramesh Chandra	Advisor, Indian Chemical Society
Professor Sunil Kumar Talapatra	Advisor, Indian Chemical Society
Professor M. C. Chattopadhyaya	Advisor, Indian Chemical Society
Professor R. N. Prasad	Advisor, Indian Chemical Society
Professor Samir Biswas	Council Member, Indian Chemical Society
Professor Ch. Venkata Ramana Reddy	Council Member, Indian Chemical Society
Professor Sheo Satya Prakash	Council Member, Indian Chemical Society
Professor Mahendra Nath Roy	Council Member, Indian Chemical Society
Professor Ranjit K. Verma	Council Member, Indian Chemical Society
Professor Anand S. Aswar	Council Member, Indian Chemical Society
Professor Ashok Kumar Mallik	Council Member, Indian Chemical Society
Professor A. D. Sawant	Editor
Dr. S. S. V. Ramakumar	IOC, Council Member (Industry)
Dr. Sanjeev Katti	ONGC, Council Member (Industry)
Dr. Md. Abdul Karim	President, Bangladesh Chemical Society, Bangladesh
Professor B. C. Ranu	Indian Association for the Cultivation of Science
Professor Sasanka Sekhar Mohanta	Head, Department of Chemistry, University of Calcutta
Professor Chiranjib Bhattacharya	Pro-Vice-Chancellor, Jadavpur University
Professor Swapan K. Bhattacharya	Head, Department of Chemistry, Jadavpur University

Organising Committee (2022)

Professor G. D. Yadav	President, Indian Chemical Society
Professor Dulal C. Mukherjee	Advisor, Indian Chemical Society
Professor Chittaranjan Sinha	Honorary Secretary, Indian Chemical Society & Convener of the Symposium
Professor Sudip Kumar Das	Honorary Treasurer, Indian Chemical Society
Dr. Nibedita Chakrabarti	Assistant Secretary, Indian Chemical Society
Professor Ayan Datta	Indian Association for the Cultivation of Science
Professor Jyotirmoyee Das	Indian Association for the Cultivation of Science
Professor Sourav Das	Department of Chemistry, Jadavpur University
Professor Surajit Chattopadhyay	Department of Chemistry, University of Kalyani
Dr. Gourisankar Roymahapatra	Haldia Institute of Technology, Haldia
Professor Debasis Mukhopadhyay	Department of Chemistry, University of Calcutta
Dr. Kamalika Sen	Department of Chemistry, University of Calcutta
Dr. Sanchita Goswami	Department of Chemistry, University of Calcutta
Dr. Tanushree Sanyal (Bala)	Department of Chemistry, University of Calcutta
Dr. Ramananda Maity	Department of Chemistry, University of Calcutta
Dr. Mijanur Rahaman Molla	Department of Chemistry, University of Calcutta
Dr. Manindranath Bera	Department of Chemistry, University of Kalyani
Dr. Chirantan Roychowdhury	Department of Chemistry, WBSUB
Dr. Soumik Bardhan	Department of Chemistry, Rampurhat College, West Bengal
Professor Md. Iqbal Rouf Mamun	General Secretary, Bangladesh Chemical Society, Dhaka
Dr. Avijit Ghosh	Heritage Institute of Technology, Kolkata

Eminent Speakers


Professor Iqbal Rouf Mamun
Secretary Bangladesh
Chemical Society,
Bangladesh


Dr. Md. Abdul Karim
President Bangladesh
Chemical Society,
Bangladesh


Prof. Krishnananda
Chattopadhyay
Indian Institute of
Chemical Biology, Kolkata


Dr. A. Vijay Kumar
ICT Mumbai

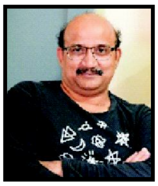

Dr. Shahid Hussain
IIT-Patna


Prof. Kumar Biradha
IIT Kharagpur


Dr. Sasmita Mohapatra
NIT Rourkela


Prof. J. J. Vittal
National University of Singapore


Prof. Debasis Mukhopadhyay
University of Calcutta


Dr. Parthasarathi Das
IIT-ISM Dhanbad


Dr. Ashwani K. Tiwari,
IISER Kolkata


Prof. Shouvik Chattopadhyay
Jadavpur University


Dr. Debasish Mandal
IIT Tirupati


Prof. Anjali Pal
IIT Kharagpur


Dr. Praveen Kumar,
IACS, Kolkata


Dr. Debayan Sarkar
IIT Indore


Dr. Dominique
Agustin, France

International Seminar on
Recent Advances in Chemistry and Material Science (RACMS-2022),
Young Scientists' Conclave (YSC-2022) & Research Scholars' Competition (RSC-2022)

PROGRAMME

30th July, 2022

Inaugural Session

Chairperson: Prof. G. D. Yadav, President
Indian Chemical Society

10:00 am	**:**	Address by Programme Coordinator
10:10 am	**:**	Welcome Address by Prof. G. D. Yadav, President, Indian Chemical Society
10:30 am	**:**	Address by Prof. C. Sinha, Honorary Secretary, Indian Chemical Society
10:40 am	**:**	Address by Prof. D. C. Mukherjee, Advisor, Indian Chemical Society
10.50 am	**:**	Inaugural Address by Prof. J. J. Vittal, Singapore
11:25 am	**:**	Vote of Thanks by Prof. S. K. Das, Honorary Treasurer, Indian Chemical Society

11:30 am – 02:00 pm
(Session -1)

Chairperson: Prof. Bimlesh Lochab
Shiv Nadar University, Uttar Pradesh

Invited Lecture 1	Dr. Dominique Agustin
Invited Lecture 2	Dr. Anukul Jana
Invited Lecture 3	Dr. Marilyn Daisy Milton
Invited Lecture 4	Dr. Nayim Sepay
Invited Lecture 5	Dr. Saifullah Lone

02:00 pm–02:30 pm: Lunch Break

02:30 pm – 06:30 pm
Parallel Session
Research Scholars' Competition

31st July, 2022

09:40 am : Address by Dr. Gourisankar Roymahapatra, Programme Coordinator
09:45 am : Address by Prof. Chittaranjan Sinha, Honorary Secretary, Indian Chemical Society

10:00 AM – 12:00 AM
(Session -1)

Chairperson: Dr. Chayan K. Nandi
IIT Mandi

4 Invited Lectures

Invited Lecture 6	Dr. Bharathwaj Sathyamooorthy
Invited Lecture 7	Dr. Tatini Rakshit
Invited Lecture 8	Dr. Thirupathi Barla
Invited Lecture 9	Dr. Ujjal K. Gautam

12:00 am – 02:00 pm
Parallel Session
Research Scholars' Competition

02:00 pm–02:30 pm: Lunch Break

02:30 pm – 03:30 pm
(Session -2)
Chairperson: Prof. Ashok K. Mallik
Council Member, ICS & Former Professor,
Jadavpur University, Kolkata

Invited Lectures

Invited Lecture 10	Dr. Sukalyan Bhadra
Invited Lecture 11	Dr. Durbadal Ojha

04:00 pm – 06:00 pm
Parallel Session
Research Scholars' Competition

06:00 pm: Vote of Thanks

August 02, 2022

: Venue :

Ramakrishna Mission Institute of Culture,
Golpark, Kolkata

Inauguration

10.00 am : National Anthem, Garlanding,
Welcome by Prof. G. D. Yadav, President, Indian Chemical Society
10.05 am : Welcome by Swami Suparnananda, Honorary Secretary, RKM Institute of Culture
10.20 am : Inauguration by His Excellency Governor, West Bengal
10.50 am : About Indian Chemical Society, Prof. D. C. Mukherjee
11.00 am : Governor Left the Dais
11.02 am : Keynote Address by Prof. Dhrubajyoti Chattopadhyay, Vice-Chancellor,
Sister Nivedita University, Kolkata
11.20 am : Chemistry, Industry and Indian Self-Reliance as visioned by Acharya Ray -
Prof. G. D. Yadav, President, ICS
11.55 am : Vote of Thanks, Prof. Sudip K. Das, Honorary Treasurer, ICS

Scientific Session – I

12.00 – 1.30 PM (Invited Lectures)

Chairperson: Prof. Samaresh Bhattacharya,
Jadavpur University, Kolkata

12.00–12.30 pm : **Invited Lecture 1**
Dr. Md. Abdul Karim, President, Bangladesh Chemical Society, Bangladesh
12.30–01.00 pm : **Invited Lecture 2** Prof. Debasis Mukhopadhyay, University of Calcutta
01.00–01.30 pm : **Invited Lecture 3** Dr. Sasmita Mohapatra, NIT Rourkela
01.30–02.30 pm : Lunch Break

Scientific Session – II

02.30–05.30 pm (Invited Lectures)

Chairperson: Prof. Tarasankar Pal, Distinguished Visiting Professor,
University of Johannesburg

02.30–03.00 pm : **Invited Lecture 4**
Professor Iqbal Rouf Mamun, Secretary, Bangladesh Chemical Society, Bangladesh
03.00–03.30 pm : **Invited Lecture 5** Prof. Kumar Biradha, IIT Kharagpur
03.30–04.00 pm : **Invited Lecture 6**
Prof. Krishnananda Chattopadhyay, Indian Institute of Chemical Biology

Chairperson: Prof. Rina Ghosh,
Jadavpur University, Kolkata

04.00–04.30 pm : **Invited Lecture 7** Dr. Shahid Hussain, IIT-Patna
04.30–05.00 pm : **Invited Lecture 8** Prof. Shouvik Chattopadhyay, Jadavpur University
05.00–05.30 pm : **Invited Lecture 9** Dr. Parthasarathi Das, IIT-ISM Dhanbad
06.00 pm : Closing

August 03, 2022

: Venue :

Dr. Triguna Sen Auditorium

Jadavpur University, Kolkata

10.00–10.05 am : Introductory Address by Prof. C. Sinha, Honorary Secretary, ICS

10.05–10.10 am : Welcome Address by Prof. Swapan K. Bhattacharya, HOD Chemistry, Jadavpur University

10.10–10.15 am : Introductory remarks by Prof. D. C. Mukherjee, Adviser, Indian Chemical Society

10.15–10.25 am : Inaugural Address by Prof. Chiranjib Bhattacharjee, Pro Vice Chancellor, Jadavpur University

10.25–10.30 am : Vote of Thanks by Prof. Saurav Das, Scientist-in-Charge, Inorganic Chemistry Section, ICS & Professor, Jadavpur University, Kolkata

Chairperson: Prof. Tapan Kanti Paine
IACS, Kolkata

10.30–11.00 am :	**Invited Lecture 10**	Dr. Ashwani Kumar Tiwari, IISER Kolkata
11.00–11.30 am :	**Invited Lecture 11**	Dr. Praveen Kumar, IACS
11.30–12.00 am :	**Invited Lecture 12**	Dr. Debasish Mandal, IIT Tirupati

Chairperson: Prof. Jhuma Ganguly,
IIEST Shibpur, Howrah

12.00–12.30 pm :	**Invited Lecture 13**	Prof. Anjali Pal, IIT Kharagpur
12.30–01.00 pm :	**Invited Lecture 14**	Dr. A Vijay Kumar, ICT Mumbai
01.00–01.30 pm :	**Invited Lecture 15**	Dr. Debayan Sarkar, IIT Indore

01.30–03.30 pm : Lunch Break & Poster Session

04.00 pm : Valedictory Session

Acknowledgement

The Indian Chemical Society thankfully acknowledges Mr. Kamalendu Ghosh, GM, SOBISCO, Eastern India for generous supply of export quality snacks for the total Program.

International Seminar on
Recent Advances in Chemistry and Material Science (RACMS-2022),
Young Scientists' Conclave (YSC-2022) & Research Scholars' Competition (RSC-2022)

The 161st Birth Anniversary Celebration of Acharya Prafulla Chandra Ray

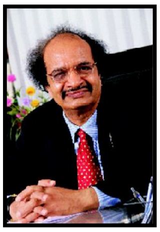
LIST OF CONTENTS

INDIAN CHEMICAL SOCIETY
92, Acharya Prafulla Chandra Road, Kolkata-700 009
Fax & Phone 91-033-23503478
E-mail:ics.correspondence@gmail.com
http://www.indianchemicalsociety.com

Professor G. D. Yadav
President

Professor Chittaranjan Sinha
Honorary Secretary

Message



Dear Delegates and attendees.

Greetings on behalf of the Indian Chemical Society which will soon celebrate the Centennial Year of its foundation. At the outset let me congratulate Hon. Smt. Doupradi Murmu, the President of India. History has been created.

On behalf of the organizing committee, we invite you to attend the International Seminar on Recent Advances in Chemistry and Material Science (RACMS-2022) as a part of the commemoration of 161st Birth Anniversary of Acharya Prafulla Chandra Ray, the Father of Indian Chemistry. The programme will be organised in two phases; at the first phase the International Research Scholars' Competition and Young Scientists' Conclave on virtual mode will be held on 30-31 July, 2022 and at the second phase off-line seminar of RACMS-2022 on 2-3 August, 2022. Nevertheless, the Council of the Society will meet in a meeting in the Library of the Indian Chemical Society Head Quarter in a programme of unveiling the statue of Acharya P. C. Ray. I am pleased to inform you that the Bangladesh Chemical Society, Bangladesh and Department of Chemistry, Jadavpur University, Kolkata are assisting in this programme.

Inauguration of 2nd August programme will be inaugurated by His Excellency, the Governor of West Bengal in the Vivekananda Hall, R. K. M. Institute of Culture, Golpark, Kolkata and on 3rd August the seminar will be held in Dr.Triguna Sen Auditorium, Jadavpur University, Kolkata.

Over the past two years, the Covid pandemic had given us new learning and new opportunity to develop dynamic digital system which improves the Global visibility of the society. The journals of the Indian Chemical Society is fully digitized and all previous issues (1924-2020) are available freely in the Society Website (www.indianchemicalsociety.com) and the journal is now published by Elsevier (2021-) and are available in the Science Direct. Our continuing efforts organise school children competition to celebrate National Science

Day (28th February); the Foundation Day (9th May) celebration brings research scholars to this platform. The carnival of Birth Anniversary of Acharya P. C. Ray (2nd August) is a yearly activity of the society and the 161st Birth Anniversary will be celebrated by different programes on 30-31 July and 2-3 August, 2022. Feature talks from leading researchers, young scientists and research scholars around the world will join both virtually and physically to celebrate this chemistry festival.

This would be a continuing event for us to pursue answers to the vital questions and learn more about the current problems related to health, education, employment, environment, energy etc. Throughout active oral and poster sessions to crosspollinate ideas and profuse opportunities to catch up with colleagues in this meeting, we will be looking back at the progression of the study during tough time for chemical research and also looking forward to the next events of the Indian Chemical Society.

GD Yadav

G. D. Yadav

President

Professor G. D. YADAV, Emeritus Professor of Eminence and Former VC, Institute of Chemical Technology, Mumbai, India

INDIAN CHEMICAL SOCIETY
92, Acharya Prafulla Chandra Road, Kolkata-700 009
Fax & Phone 91-033-23503478
E-mail:ics.correspondence@gmail.com
http://www.indianchemicalsociety.com

Professor G. D. Yadav
President

Professor Chittaranjan Sinha
Honorary Secretary

Message

It is a matter of great pleasure that the Indian Chemical Society has ventured to celebrate the 161st Birth Anniversary of Acharya Prafulla Chandra Ray, the doyen of chemical sciences in India, by organizing Research Scholars' Competition followed by the International Seminar during July 30-31 and August 02-03, 2022 in association with the Bangladesh Chemical Society, Bangladesh and the Department of Chemistry, Jadavpur University, Kolkata.

It is my proud privilege to bring to the notice of all concerned that the Indian Chemical Society, since its foundation in 1924, has been continuously striving for generation and dissemination of knowledge of Chemical Science and Technology throughout the entire world. Being inspired by a nationalist spirit - J. N. Mukherjee, J. C. Ghosh, S. S. Bhatnagar, N. R. Dhar and other distinguished contemporaries took an undaunted endeavour to establish the Indian Chemical Society with Acharya Prafulla Chandra Ray as its founder president. At a later stage, the Society received the scholastic services of Priyadaranjan Ray, B. C. Guha, P. B. Sarkar, B. N. Ghosh, Jagdish Shankar, T. R. Seshardri, R. C. Mehrotra, Sukh Dev, T. R. Govindachari, Sushil K. Mukherjee and some other stalwarts in the field of chemical science in our country.

A linguist, having proficiency in major languages of the world and a voracious reader of literature, Prafulla Chandra was the founder of Indian School of Modern Chemistry and a pioneer of chemical industries in India. By leading a simple life of ascetic self-denial, by his patriotism, philanthropy and entrepreneurship and also with his erudition and wisdom Prafulla Chandra had set up a transcendental idealism to be cherished by his countrymen from generation to generation.

I presume that some basic issues of global interest would find place in the deliberations and I hope that new ideas will emanate and new directions of future research will be indicated in the international seminar.

The organising committee of this International Seminar deserves applause and appreciation for undertaking the commendable task of organising such an important event.

I wish the Event a grand success.

Dulal C. Mukherjee

Professor (Retd.) of Chemistry,
University of Calcutta
& Advisor, Indian Chemical Society

INDIAN CHEMICAL SOCIETY
92, Acharya Prafulla Chandra Road, Kolkata-700 009
Fax & Phone 91-033-23503478
E-mail:ics.correspondence@gmail.com
http://www.indianchemicalsociety.com

Professor G. D. Yadav
President

Professor Chittaranjan Sinha
Honorary Secretary

Welcome Address

Welcome to 161st Birth Anniversary Celebration of Acharya P. C. Ray

It gives me immense pleasure to inform you that the Indian Chemical Society (ICS) shows her indomitable spirit throughout the Covid 19 for long two years of lockdown massacre period. Since March 2020 to July 2022 the ICS organised as many as ten national seminars, four international seminars, six lectureship programes, two internship events for long 8 weeks at every week end (Saturday & Sunday) and most importantly 57th and 58th Annual Convention of Chemists. Although we were depressed due to sad demise of our beloved Shibuda, retired staff, Mr. S. N. Dewan on 8th April just one month before the 99th Foundation Day celebration on 9th May, 2022 but the activities of the Society continues. As a part of popularization of chemistry through arranging seminars, symposia, science competitions, publishing Books, periodicals etc. the Society is arranging the commemoration of 161st Birth Anniversary Celebration of Acharya P. C. Ray, Father of Indian Chemistry and First President of the Indian Chemical Society (1924), through International Research Scholars' Competition (on-line) on 30-31 July, 2022 followed by International Seminar on Recent Advances in Chemistry and Material Science-2022 (RACMS-2022) by physical mode on 2-3 August, 2022. I am happy to share that the program is collaborated first time with Bangladesh Chemical Society (BCS) in association with the Department of Chemistry, Jadavpur University, Kolkata.

The purposeful events help to blossom creativity, emanate thinking which assist to lit knowledge and knowledge is responsible to ignite minds. An ignited mind is the most powerful resource on earth, above the earth, and under the earth. This is what discoverer of Mercurous Nitrite, Author of 'A History of Hindu Chemistry' and Founder of first Private Pharma-Industry in British ruled India, Bengal Chemical and Pharmaceutical Works Ltd. dreamed in his dream and the Indian Chemical Society brings it in reality.

International Research Scholars' Competition (on-line) on 30-31 July, 2022 will be inaugurated by Emeritus Professor, Prof. J. J. Vittal, a Crystal Engineer & Material Scientist, NUS, Singapore in presence of Padma Shree Prof. G. D. Yadav, President, ICS. More than 150 Research Scholars will join in the competition along with 12 speakers in Young Scientists' Conclave. There are seventeen speakers in the Recent Advances in Chemistry and Material Science-2022 (RACMS-2022) on 2-3 August, 2022 (physical mode). 1st August is the day where a statue of Acharya Ray will be unveiled in the Library of the Society by Prof. Animesh Chakravorty, a passionate admirer of Acharya Ray.

All the members, well-wishers and scientists are welcomed in this program to commemorate 161st Birth Anniversary of Acharya P. C. Ray.

With regards.

Yours sincerely

Chittaranjan Sinha

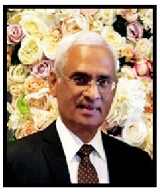
Professor Chittaranjan Sinha
Honorary Secretary
Indian Chemical Society

Invited Lectures

[1 – 25]

Inagural Address

Invited Lecture-1



Attributes of successful researchers and great scientists

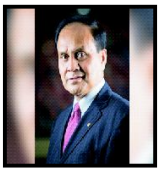
Jagadese J. Vittal
Department of Chemistry,
National University of Singapore,
Singapore
E-mail: jjvittal@nus.edu.sg

In this busy world, competition becomes an inevitable and part of any career. Research field is no exception. As a young researcher and scientist, we always wonder how we can be successful in our chosen career. As an aspiring researcher, we expect to have love of science, child-like curiosity, creative thinking, imagination & dream, motivation, inspiration, dedication, etc. Further, not afraid of failing mentality, never give-up attitude, open mind to fresh ideas (*Think outside the box*), presentation and communication skills, never compromise habit, critical thinking will help in achieving our dream. It is also essential to practice ethics in our research. Researchers are also responsible for the reliability and reproducibility of their data. The talk will highlight a few aspects of these attributes and intend to motivate the young scientists and research scholars to be successful researchers.

Brief Bio-Sketch

Jagadese J. Vittal obtained PhD from Indian Institute of Science, Bangalore (1982). He was a postdoctoral research associate and a service crystallographer at the University of Western Ontario, Canada before moving to the National University of Singapore as a faculty member in 1997. He is an Emeritus Professor from 2021. J. J. is interested in solid state science and structural chemistry including new materials, chemical reactivities, and structure-property relationships. He was the founding member of *Singapore National Crystal Growing Challenge* and co-authored a textbook on Crystal Engineering and edited two books.

Invited Lecture-2



Science education and research in Bangladesh: Problems and prospects

Md. Abdul Karim
President, Bangladesh Chemical Society
E-mail: akarim521@gmail.com

A knowledge-based society based on education and research was the dream of Bangladesh's founding father Bangabandhu Sheikh Mujibur Rahman. This paper focuses on the current state of Science Education and Research in Bangladesh with few policy recommendations for future improvement of the scenario. Acharya Prafulla Chandra Roy, the "Revolutionary in the grab of a Scientist" is the father of Chemistry education and research in undivided India. Chemistry research was pioneered in then Pakistan by eminent educationist Dr. Qudrat -E-Khuda who established Pakistan Council of Scientific and Industrial Research (PCSIR) (now BCSIR) and headed the country's fast Education Commission. Mukaram Hossain Khandoker played important role in the spread of Chemistry education in Bangladesh. Significant success was achieved in this regard. However, in recent years, a number of factors including insufficient allocations in the national plans/budgets and reluctance of many students to study science has recently resulted in limited success of scientific research in Bangladesh. In a typical private university, more than 50% of the students are now enrolled in Bachelor of Business Administration (BBA) courses due to the job market demand mostly in the multinational companies. MNCs tend to recruit sales agents rather than encouraging research based intellectual society. Moreover, the focus on science education and research in various development plans of Bangladesh seem insufficient although the 20-year Perspective Plan (2021-2041) emphasizes that the entire education system has to be redesigned to move from factor driven stage to innovation-based economy. The country's plans need to allocate enhanced resources for education and research. Chemical laboratories need to be well modernized and appropriately equipped. The recommendations of this paper may significantly contribute to the development of Bangladesh by creating knowledge-based society and achieve its SDG Goals.

Brief Bio-Sketch

Dr. Md. Abdul Karim, Executive Director of UCEP Bangladesh brings 44 years of experience in the Field Administration, Foreign Missions, Secretariat, NGO, and Corporate sectors. He is the President of Bangladesh Chemical Society, Bangladesh Scouts Foundation, Bangladesh Deaf Sports Federation and Chittagong University Alumni Association. He is the Advisory Board Member of the Asian University for Women (AUW), Chattogram.

Mr. Karim previously served as Secretary to the Government of Bangladesh in the Ministry of Home Affairs, Commerce, Fisheries and Livestock, Finance (Internal Resources Division) and Communications (Bridges Division) before becoming the Principal Secretary. He was Chairman of National Board of Revenue (NBR); President of Bangladesh Scouts, Managing Director of Palli Karma-Sahayak Foundation (PKSF) and Senior Advisor of BRAC.

Dr. Abdul Karim was educated at the University of Chittagong and the University of Birmingham, UK. He obtained PhD from Bangladesh University Professionals (BUP), Dhaka. He travelled to 60 countries and represented Bangladesh in many international Fora, Conferences and Summits. He has written books and articles on local government, environment, poverty reduction, empowerment of women and the elderly, disaster management etc. Dr. Karim has lectured at North South University, State University of Bangladesh, University of Liberal Arts of Bangladesh (ULAB), Public Administration Training Centre, Bangladesh Military Academy, National Défense College, Bangladesh Civil Service (Administration) Academy etc. Mr. Karim has received the highest Scout Award of Bangladesh. Dr. Karim spoke on the Anti-Terrorism Policy and Money Laundering Prevention Policy of Bangladesh at the Pentagon, US State Department, Justice Department, Federal Reserve etc in 2009.

Invited Lecture-3

Food safety management in Bangladesh: Challenges and way forward

Md. Iqbal Rouf Mamun
Department of Chemistry,
University of Dhaka,
Bangladesh
E-mail: iqbalrouf@yahoo.com

In common with many countries in the region, food safety control in Bangladesh has traditionally been the responsibility of a number of central government organisations such as the ministries or departments of agriculture, health, trade and commerce. At local level these responsibilities are delegated to local authorities, municipalities or local governments. A weakness in our current system of food control is that collaboration and cooperation between the various government organisations are very poor or absent. Effective food safety control is undermined by the existence of fragmented legislation, multiple jurisdictions, and inconsistencies in enforcement and weaknesses in food surveillance and monitoring.

In recent years, major government initiatives are underway in Bangladesh to strengthen the national food control system and improve inter-ministerial agency collaboration in the area of food control for the protection of consumer health and facilitation of food trade. Bangladesh Food Safety Authority (BFSA) has been established in 2015 under The Food Safety Act 2013 as a central competent authority to regulate, through coordination, all activities relating to food production, import, processing, and marketing. The BFSA is tasked with coordinating official food controls across the food chain; working in collaboration with government agencies responsible for food inspection; setting food standards; providing scientific advice to strengthen food safety policy; and developing and disseminating food safety training and awareness materials. This presentation will discuss recent developments, challenges and way forward to an effective food control system in Bangladesh.

Brief Bio-Sketch

Dr. Md. Iqbal Rouf Mamun, is a Professor of Chemistry at the University of Dhaka, Bangladesh. Secured his position as a Lecturer of the University of Dhaka in 2000 be successfully elevated to the position of Professor in 2013. Prof. Mamun has vast research experience both in 'Natural Product

Chemistry' and 'Chemical Contaminants in Food & Environment'. Research involves chemical & biological studies of medicinal plants, analysis of persistent organic pollutants in food and environmental samples, method development for determination of antibiotic residues in food, determination of pesticides residues in fruits & vegetable. He pursued PhD degree in 1999 from the University of Dhaka with financial support from the International Science program (ISP), Sweden and did Post-Doctoral research in Chonnam National University, Republic of Korea. Having credits of 54 scientific papers published in national and international journals, he has been one of the Founder Members of Bangladesh Food Safety Authority (BFSA) during 2015-2019. Currently, he is the General Secretary of Bangladesh Chemical Society (BCS), Chairperson of Sweden Alumni Network Bangladesh (SANB) and a member of Reviewer's Panel of several reputed international journals related to food and environment. He has attended more than 100 scientific seminars/conferences and presented his research works.

Invited Lecture-4

Fishing out a colon cancer biomarker, Hyaluronan with correlative AFM and Spectroscopy

Tatini Rakshit
Department of Chemistry,
Shiv Nadar University,
Delhi-NCR, India
E-mail: tatini.rakshit@snu.edu.in

Extracellular vesicles (EV) are naturally occurring nanoparticles with unique structure, surface biochemistry, and mechanical characteristics. These distinct nanometer-sized bio-particles are secreted from the surfaces of normal and cancer cells and are of potential interest as cancer biomarkers[1]. We use high-resolution Atomic force Microscopy (AFM) to show single-vesicle quantitative differences between EVs derived from colon cancer cell HCT 116 and normal colon epithelial cell CCD-Co18. At the single-vesicle level, HCT 116 derived EVs exhibit significantly ($P < 0.05$) increased Hyaluronan surface densities compare to CCD-Co18. Spectroscopic experiments including Fourier Transform Infrared Spectroscopy (FT-IR), Circular Dichroism (CD) and RAMAN spectroscopy univocally support our observation[2]. Taken together, this strategy could be realized as a non-invasive colon cancer diagnostic in future.

References

1. K. Rilla, H. Siiskonen, M. Tammi and R. Tammi, *Advances in Cancer Research*, 2014, **123**, 122.
2. D. Paul, A. Roy, B. Dutta, A. Roy, P. Borar, S. K. Pal, D. Senapati and T. Rakshit, *Journal of Physical Chemistry Letters*, 2020, **11**, 5569.

Brief Bio-Sketch

Dr. Tatini Rakshit obtained her BSc and MSc in Chemistry from Jadavpur University. Then, she joined Indian Association for the Cultivation of Science, Kolkata for her doctoral studies. After completing the thesis work on “Tunable Ferritin Bioelectronics at the Nanoscale” Dr. Rakshit moved to a post-doctoral position at Case Western Reserve University, Ohio. She completed another post-doctoral stint at the National Cancer Institute, NIH, MD before joining S. N. Bose National Centre for Basic Sciences, Kolkata as a DST Inspire Faculty fellow. Recently she joined Shiv Nadar University, Delhi as an Assistant Professor. Her primary research focus includes bioanalytical chemistry, biosensing and bioimaging.

Invited Lecture-5

To restart or not? - Stochastic resetting in drift-diffusion processes

Debasish Mondal
Department of Chemistry and Center for Molecular
and Optical Sciences & Technologies,
Indian Institute of Technology Tirupati,
Yerpedu-517 619, Andhra Pradesh, India
E-mail: dmondal@iittp.ac.im

Restart plays a central role in shaping the completion time in a stochastic search process. First passage processes can either be accelerated by the introduction of restart or can display an opposite response. We explore a transition between these two classes by varying governing parameters. We quantify the effect of stochastic restart (SR) on the first-passage time of a drift-diffusion process to an absorbing boundary. We explore that the transition is governed by the relative dominance between the adjective rate and the diffusive transport (Peclet number). The transition considered herein stands at the core of restart phenomena and is relevant to a large variety of processes with unique characteristics. As an interesting example of SR in a Drift-diffusion process, we describe the effect of an asymmetric SR in a stochastic climate model. The theoretical perspective provides a roadmap to prevent the abnormal precipitation accumulation caused by the global warming.

References

1. M. R. Evans and S. N. Majumdar, Diffusion with stochastic resetting, *Phys. Rev. Lett.,* 2011, **106**, 160601.
2. S. Ray, D. Mondal and S. Reuveni, Peclet number governs transition to acceleratory restart in drift-diffusion. *J. Phys. A: Math. Theor.*, 2019, **52**, 255502.
3. S. Y. Ali, N. Choudhury and D. Mondal, Asymmetric restart in a stochastic climate model: A theoretical perspective to prevent the abnormal precipitation accumulation caused by global warming, *J. Phys. A: Math. Theor.,* 2022, **55** 301001.

Brief Bio-Sketch

Dr. Debasish Mondal did his doctoral research under the supervision of Professor Debshankar Ray, Indian Association for the Cultivation of Science and received his PhD degree from the University of Calcutta in 2012. He was also the recipient of the Sir P. C. Ray Research Award in the year of

2011 awarded by Indian Chemical Society and the University of Calcutta. He pursued his postdoctoral research works at Virginia Tech. USA, University of Massachusetts Amherst, USA and Leibnitz Institute for Polymer Research, Germany. Dr. Mondal joined Indian Institute of Technology Tirupati as an Assistant Professor in 2017. His broad research interest covers wide range of nonequilibrium statistical mechanics that explore effect of the thermal fluctuations in different Biophysical processes at the macromolecular level. In particular he is working on polymer translocation process, stochastic resetting phenomena and Brownian information engines.

Invited Lecture-6

Synthetic studies towards dibenzobicyclo[3.2.1]-octadienone containing natural products

Barla Thirupathi
Department of Chemical Sciences,
Indian Institute of Science Education and Research Berhampur,
Berhampur
E-mail: thirupathibarla@iiserbpr.ac.in

The dibenzobicyclo[3.2.1]octadienone scaffold, which has been found in naphthocyclinones, engelharquinones, rubialatin A, etc., (Fig. 1)[1]. Most of these natural products exhibit a wide variety of biological activities such as antibacterial, antitumor, antifungal, and cytotoxic properties. We have developed a mild, transition-metal-free, synthetic strategy to access the challenging dibenzobicyclo[3.2.1]octadienone scaffolds by aryne insertion

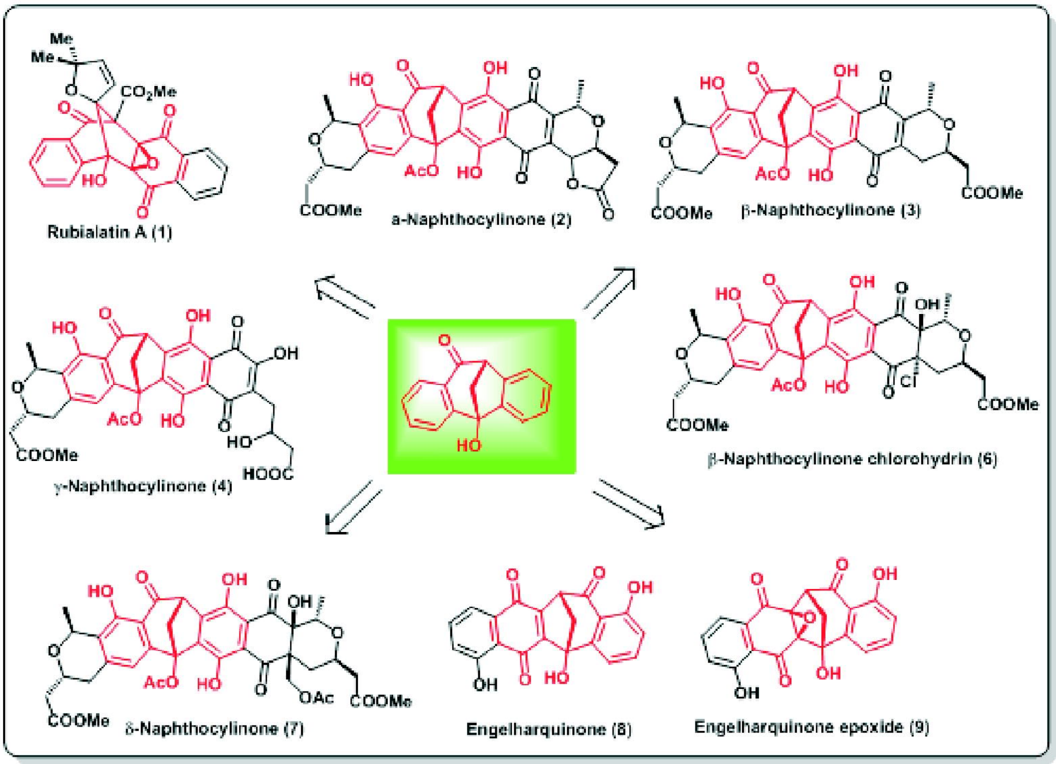


Fig. 1. A few natural products bearing dibenzobicyclo[3.2.1]octadienone scaffold.

reaction with 2-keto-1,3-indandiones.[2] The foremost advantages of the protocol are direct access to 4 to 5 fused rings containing dibenzobicyclo[3.2.1]octadienone scaffolds as well as the tolerance of various functional groups. Application of this strategy has been demonstrated to the synthesis 6/6/5/6/6 dibenzobicyclo[3.2.1]octadienone skeleton of a rubialatin A. The simple reaction conditions and flexible synthetic strategy offer a unique path to the total synthesis of unaccomplished targets, (α-δ)-naphthoquinones, and other related natural products. ^{1}H-NMR experimental studies suggested this reaction proceeds through benzocyclobutane formation followed by a 7-membered carbocycle ring[2].

References and Notes

1. (a) S. Kamo, K. Kuramochi and K. Tsubaki, *Tetrahedron Letters,* 2018, **59**, 224-230;
   (b) R. A. Fernandes, P. H. Patil and D. A. Chaudhari, *Eur. J. Org. Chem.*, 2016, **2016**, 5778-5798.
2. G. Hazra, G. Mishra, R. Dandela and B. Thirupathi, *The Journal of Organic Chemistry,* 2022. doi: 10.1021/acs.joc.2c00340.

Brief Bio-Sketch

Dr. Thirupathi Barla was born in Madavelli, Manchirial district, Telangana, India in 1984. After completion of M.Sc. (Organic Chemistry) from Osmania University (2006-2008), he worked as a research chemist at GVK-Biosciences, Hyderabad (2008-2009). In early 2009 he joined as Junior Research Fellow (JRF) at CSIR Indian Institute of Chemical Technology, Hyderabad with Dr. D. K. Mohapatra for doctoral studies (2009-2014). Afterward, he worked as an associate research scientist in-process R&D division at Sai Life sciences, Hyderabad (2014-2015). Then Dr. Barla moved to Harvard University as a postdoctoral fellow to work with Prof. E. J. Corey (2015-2018) where he involved in the development of highly active fluorinated second generation oxazaborolidine catalysts and their application in Diels-Alder reactions. In July 2018, he became an Assistant Professor of Chemistry at the Indian Institute of Science Education and Research Berhampur. Dr. Thirupathi's area of research includes the total synthesis of biologically active natural products or model compounds having potential bioactivities. Dr. Thirupathi's group also works on the development of novel carbon-corban bond formation reaction and their application towards natural products synthesis.

Invited Lecture-7

Study of nonadiabatic effect on dissociation channels of HCNH – the issue of abundance ratio [HNC]/[HCN] in the upper atmosphere

Debasis Mukhopadhyay
Department of Chemistry,
E-mail:

Theoretical Chemists, mostly rely on the adiabatic description of molecular structures and dynamics, based on the separation of fast moving light electrons and slow moving heavy nuclei (Born-Oppenheimer (B.O) approximation). However, there are several processes, known as electronically non-adiabatic processes, e.g. photochemical and photobiological processes, radiationless decay of excited electronic states, isomerization processes of polyatomic molecules, photoinduced unimolecular decay, inelastic atom-atom or atom-molecule collisions etc., which can't be explained by this framework. For a polyatomic molecule (not for a diatomic molecule) two adjacent adiabatic states may be degenerate for a particular nuclear configuration space and for such cases nuclear motion can't be restricted to a single surface; the coupling between two adjacent states i.e. non adiabatic coupling term become large enough, and therefore the ordinary B.O approximation may breakdown. In the present lecture we are taking the non-adiabatic effects in low-lying electronic states of HCNH, the precursor molecular system for HCN and HNC, as a probe to explain the abnormal abundance of HNC in interstellar spaces, while highly correlated ab initio molecular orbital calculations show that HNC is much less stable than HCN.

Brief Bio-Sketch

Debasis Mukhopadhyay is a Professor in Physical Chemistry in University of Calcutta. He is in teaching profession since April, 1992, first as a Lecturer in Chemistry in Ramakrishna Mission Vidyamandira, Belur Math till September, 2005 and then as a Professor in Chemistry in University of Calcutta till date. From the viewpoint of research activities, Professor Mukhopadhyay is a theoretical Chemist with research interest in molecular electronic structure theory and electronic non-adiabatic interactions. He has co-authored more than 35 research publications in various journals of international repute. He has completed his Bachelor of Science with honours in chemistry and Masters in Chemistry from the University of Burdwan. In various phases of his research carrier he has worked (visited) in Indian Association for the Cultivation of Science, Kolkata (as a PhD student and thereafter), Princeton University(USA), Institute of Molecular Science (Japan) and the University of Tokyo (Japan).

Invited Lecture-8

Metal chalcogenide nanomaterials for photocatalytic and adsorption applications

Sahid Hussain
Department of Chemistry,
Indian Institute of Technology Patna,
Patna, India
E-mail: sahid@iitp.ac.in

Green Chemistry has received intense attention both in academia and industry. The manufacturing processes in the industry may involve hazardous steps or inputs and may not be eco-friendly. The future, therefore, depends on how we cope with this situation. Green Chemistry seems to be the only option for long-term sustainability. Key principles of green chemistry encompass the design of safer molecules, the use of less hazardous and energy-intensive synthetic routes, safer solvents, and to treat the toxic waste.

Photocatalysis and adsorption by nanoscale material are the areas that attracted great interest due to their potential applications in the areas of environmental and energy issues. TiO_2 was the first semiconductor photocatalyst that was applied and was only active under ultraviolet light due to its wide band gap[1]. In order to utilize the solar spectrum of the desired wavelength, tailoring of the band gap is invoked as one of the effective techniques. One of the current challenges is to synthesize photocatalysts with desired band gap via a novel and benign protocol with controlled shape and size. On the other hand, adsorption is a non-destructive technique for the removal of dyes from wastewater. In order to have adsorption, the material should have a surface with charge, pores, or functional group that leads to electrostatic interaction, ionic exchange, hydrogen bonding, and coordination with metal.

Scheme 1. Organic dye adsorption and degradation by metal chalcogenides.

We present here the environmentally benign route for the synthesis of binary and multinary chalcogenides like NiS[2], Bi–In–Zn–S (BIZS)[3], Ag–In–Ni–S[4], CoS[5] and Ni-Co-S[6] with controlled phase and tunable band gap. Band gap and surface charge are tuned by varying the ratio of metals and chalcogens. The band gap and surface charge were evaluated for these multicomponent chalcogenide nanocrystals (MCNs) and was found that these nanocrystals were active for both adsorption and photodegradation. It is anticipated that adsorption and photodegradation can find practical applications in wastewater treatment targeting the colored effluents of the dye industries.

References

1. A. Fujishima and K. Honda, *Nature*, 1972, **238**, 37.
2. A. Molla, M. Sahu and S. Hussain, *Sci. Rep.*, 2016, **6**, 26034.
3. A. Molla, M. Sahu, Y. Kumar and S. Hussain, *RSC Adv.*, 2015, **5**, 41941.
4. A. Molla, M. Sahu and S Hussain, *J. Mater. Chem. A*, 2015, **3**, 15616.
5. A. A. Khan, S. Kumari, A. Chowdhury and S. Hussain, *ACS Appl. Nano Mater.*, 2018, **1**, 3474.
6. A. Chowdhury, A. A. Khan, S. Kumari and S. Hussain, *ACS Sustainable Chem.& Eng. Chem. Eng.,* 2019, **7**, 4165.

Brief Bio-Sketch

Dr. Sahid Hussain, born on 10 February 1978 in Bihar, obtained a master’s degree in chemistry from Cotton College, Guwahati (Gauhati University) in 2002. He secured a PhD from IIT Guwahati in 2008 and moved to the Pohang University of Science and Technology, South Korea for his Postdoctoral Research. He returned to India to join the IIT Patna as Assistant Professor in December 2008. He is currently serving as an Associate Professor in the Department of Chemistry and his current research interests are the development of new organic synthetic methodologies, nanoscale materials for photocatalysis and adsorption, and multicomponent reactions. He has 4 patents and 60 journal publications of repute to his credit.

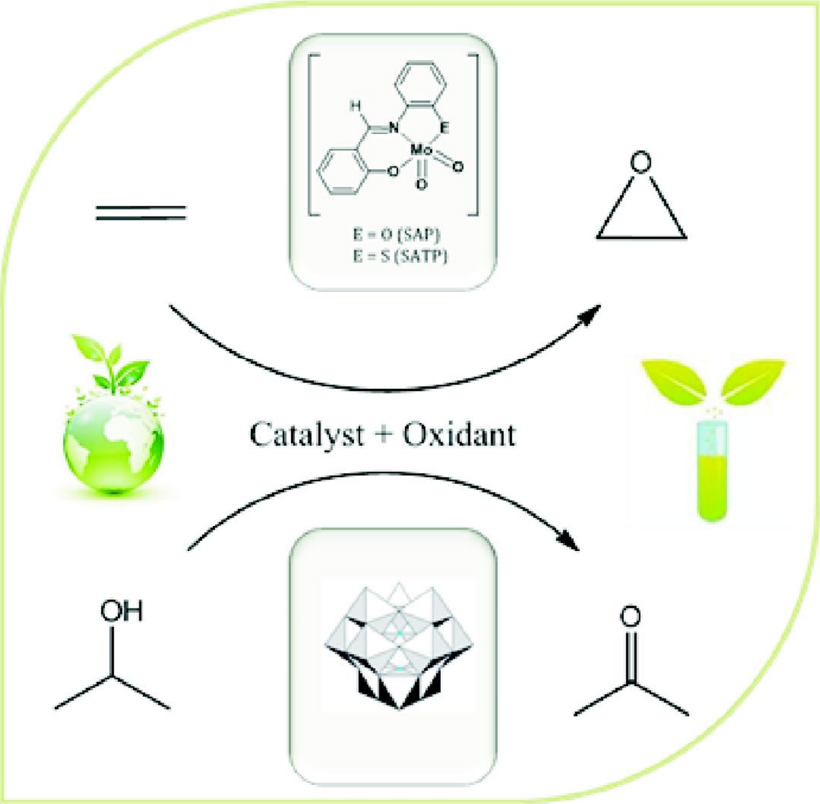
Invited Lecture-9

"Greener" Metal-catalyzed(ep)oxidation

Dominique Agustin
Université de Toulouse,
Institut Universitaire de Technologie Paul Sabatier,
Département de Chimie, Av. Georges Pompidou,
BP 20258, 81104 Castres, France

CNRS, LCC, Université de Toulouse, UPS,
INPT, 205, route de Narbonne, 31077 Toulouse, France
E-mail: dominique.agustin@iut-tlse3.fr

Catalysis is one important aspect of the Green chemistry principles, being an interesting eco-logical and eco-nomical concept. Since many classical procedures use stoichiometric amounts of non-green oxidants and hazardous organic solvents/reagents, catalyzed organic solvent-free processes and/or grafted catalysts have been increasing.



We work on organic solvent-free epoxidation of olefins catalyzed by metal complexes or Keggin-based polyoxometalates. One aim of the present work is to study experimentally and through DFT calculations the influence of modified SAP ligands towards the activity of the related molybdenum complexes in the epoxidation of cyclooctene by aqueous tert-butyl hydroperoxide (TBHP).

Another aim is to support the catalyst (on Merrifield resin or functionalized silica beads) to recycle catalytic objects. Synthetic procedures, catalytic results and valorization of the process by transformation of natural products will also be shown.

Brief Bio-Sketch

Dominique Agustin is Associate Professor. He teaches at Chemistry Department of Technological University Institute of the Université Paul Sabatier (Toulouse 3) and conducts his research within the LAC2 research team at “Laboratoire de Chimie de Coordination” of CNRS. Teaching and Research are done in Castres (Tarn)

He did his B.S in Chemistry at Université Perpignan then all the rest of studies at Université Paul Sabatier until PhD in 1999. After 3 years post-doc at University of Saarland (Germany), he was appointed as assistant Professor at Sorbonne University in 2002 then moved to Castres in 2006.

Within the frame of Sustainable Chemistry, his research concerns biomass valorisation using catalysed processes under clean and atom-economic conditions, as well as the reasoned use of resources within the context of a circular economy.

Dominique Agustin is implied within science popularisation as co-pilot of a series of scientific meetings in Castres (rencontres Exploreur – Sciences en circuit court) and personally presenting in several events as “Fête de la Science”.

He is also dedicated to the French Scientific Community as Secretary of the Sustainable Chemistry Division of the French Chemical Society.

Invited Lecture-10

Reuse and Recycle: A green chemistry approach

Anjali Pal
Department of Civil Engineering,
Indian Institute of Technology Kharagpur,
Kharagpur-721 302, West Bengal
E-mail: anjalipal@civil.iitkgp.ac.in

Chitosan (CS) hydrogel beads are extensively used for metal ion removal from aqueous solution. CS gel beads are modified using sodium dodecyl sulfate (SDS), which is an anionic surfactant, with formation of a bilayer (admicelle) on to it. The SDS concentration used for the modification of CS gel beads is 6000 mg/L. These surfactant-modified CS gel beads are named as POSTCS beads. Next Ni(II) is loaded on the SDS bilayer through a process known as 'adsolubilization'. The Ni(II) loading is about 4 times higher in POSTCS beads compared to that in normal CS beads. In the next step Ni@NiO core-shell nanoparticles are formed on POSTCS beads by borohydride reduction. The as-prepared particles show excellent catalytic properties toward 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) reduction in presence of borohydride. The reaction follows first order rate. The turn over number (TON) and turn over frequency (TOF) have been calculated. The as-prepared catalyst shows activity comparable to other catalysts. This way CS, which is a marine waste, could be used for surfactant removal, Ni(II) removal from polluted water, and finally the waste adsorbent could be transformed in to a catalyst for 4-NP reduction.

Brief Bio-Sketch

Dr. Anjali Pal, M.Sc, PhD is a chemistry graduate from the University of Calcutta and at present is a professor in the Department of Civil Engineering, Indian Institute of Technology (IIT) Kharagpur. Dr. Pal is actively engaged in teaching and research in the field of environmental engineering and science. She has published more than 230 research papers and supervised 12 students for PhD program. Her fields of research involves speciation of arsenic, modified Fenton and photo-Fenton reactions, photocatalysis, and catalysis with metal nanoparticles, adsolubilization process, and spectroscopy. Wastewater remediation by new adsorption technology for 'zero waste' technology is now her 1st priority for field application. Dr. Pal has received convention award from the Indian Chemical Society, International Hall of Fame award and R & D-100 award from USA. She has visited many countries as a visiting professor.

Invited Lecture-11

MOFs as heterogeneous catalysts for water splitting and chemical fixation of CO_2

Kumar Biradha
Department of Chemistry,
Indian Institute of Technology Kharagpur,
Kharagpur-721 302, India
E-mail: kbiradha@yahoo.com

Supramolecular Chemistry and Molecular Crystal Engineering are two powerful weapons for chemists in designing highly crystalline and porous supramolecular polymeric architectures with desired physical and chemical properties[1,3]. Metal-organic frameworks (MOFs) represent a special class of hybrid inorganic-organic porous supramolecular materials consisting of metal containing clusters (usually known as secondary building units (SBUs)) and organic ligands (referred as “struts”) through strong coordination bonds (recognised as “reticular synthesis”) to generate open pore frameworks with permanent porosity, high thermal stability and enormous scope of tunable functional properties[4,5]. MOFs symbolize the beauty with brilliant chemical structures having framework flexibility. Thus, the modular nature and facile tunability of MOFs make them ideal candidates for heterogeneous catalysis with uniform active sites through judicial choice of building blocks. In catalysis, MOFs allow to overcome the primary limitations of discreet metal complex based homogeneous catalysis and single atom catalysts (SACs) owing to MOFs heterogeneous nature and easier separation technique with structural tuning and refinement, while their ultrahigh surface area, pore volume, and heterogeneous nature facilitate the maximum exposure of catalytic active centres. The post synthetic transmetallation and solvent assistable linker exchange of MOFs could also result a new daughter MOF with better stability and properties than the parent one which otherwise can’t be obtained.

With the well anticipation and rapid enhancement in zero emission energy technology, hydrogen is one of the cleanest next generation energy materials having its high energy density (120 *vs* 44 MJ Kg^{-1} for gasoline), high combustion efficiency, and non-toxic nature. The electrochemical overall splitting into hydrogen and oxygen ($2H_2O \rightarrow 2H_2+O_2$) can be an effective and promising approach for large-scale hydrogen fuel production with high purity and no emission towards next generation energy technologies such as metal-air batteries, and proton exchange membrane fuel cells (PEMFC)[6]. On the other hand, the atmospheric CO_2 which is a major component of green house effect and responsible for global warming can often be explored and utilized as a C1- building block for organic synthesis by its catalytic fixation from atmosphere. The chemical fixation of CO_2 by the epoxides into cyclic carbonates is a 100 % atom economical process. Thence, there is urgent and crucial need to fabricate robust, and cost-effective earth abundant transition metal containing MOF based heterogeneous catalysts for high performance overall water splitting and chemical conversion of atmospheric CO_2. The recent perspective article by Yang and Wang and their co-workers have been generalized by a vivid discussion on design strategies for recent heterogeneous MOF based electrocatalysts for water splitting and CO_2 fixation[7]. In our recent feature article, we also have briefly summarized the engineering strategies and composition-structure-activity relationships for the pristine MOF based materials for such heterogeneous catalytic applications[8]. In summary, the field of MOF based heterogeneous catalysis towards energy conversion and storage technology is a fast growing, impactful and diversified field of research for comprehensive understanding of the catalytic process at atomic and supramolecular level for the sustainable development of mankind.

References

1. J.-M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives* VCH, Weinheim, 1995.
2. J.-M. Lehn, Supramolecular chemistry-scope and perspectives molecules, supermolecules, and molecular devices (Nobel Lecture). *Angew. Chem., Int. Ed. Engl.,* 1988, **27**, 89-112.
3. G. R. Desiraju, Crystal Engineering; from molecule to crystal. *J. Am. Chem. Soc.*, 2013, **135**, 9952-9967.
4. K. Biradha, A. Ramanan and J. J. Vittal, Coordination polymers versus metal-organic frameworks, *Cryst. Growth Des.*, 2009, **9**, 2969-2970.
5. M. J. Kalmutzki, N. Hanikel and O. M. Yaghi, Secondary building units as the turning point in the development of the reticular chemistry of MOFs, *Sci. Adv.*, 2018, **4**, eaat9180.
6. M. G. Walter, E. L. Warren, J. R. McKone, S. W. Boettcher, Q. Mi, E. A. Santori and N. S. Lewis, *Chem. Rev.*, 2010, **110***,* 6446-6473.
7. P. -F. Zhang, D. Wu, G. -P. Yang and Y. -Y. Wang, Metal-Organic frameworks as heterogeneous electrocatalysts for water splitting and CO_2 fixation. *Cryst. Growth Des.*, 2021, **21**, 3123-3142.
8. K. Biradha, A. Goswami and R. Moi, Coordination polymers as heterogeneous catalysts in hydrogen evolution and oxygen evolution reactions. *Chem. Commun.*, 2020, **56**, 10824-10842.

Brief Bio-Sketch

Kumar Biradha received his Ph.D. in Chemistry from the University of Hyderabad, Hyderabad, India in 1997. Subsequently he did his post-doctoral research in Saint Mary's university, Halifax, Canada and Nagoya University, Nagoya, Japan. Currently he is working as a Professor at the Indian Institute of Technology, Kharagpur, India. He is the author of over 200 research publications which covers his research interests in supramolecular chemistry, crystal engineering, solid state reactions, MOFs, gels and materials chemistry. He served as editorial board member of *New Journal of Chemistry*, *R. Sc*. (2008-2011) and served as co-editor for *Acta Cryst. Sec-E* (2011). He worked as Associate Editor of *Crystal Growth & Design*, ACS publications for 10 years (2012-2021) and member of research council of CSIR-NEIST, Jorhat, India (2017-2020).

Invited Lecture-12

Multi-stimuli responsive fluorochromic switching in phenothiazine derivatives

Marilyn Daisy Milton
Functional Organic Molecules Synthesis Laboratory,
Department of Chemistry,
University of Delhi,
Delhi-110 007, India
E-mail: mdmilton@chemistry.du.ac.in

Stimuli-responsive materials undergo reversible transformation in response to external stimuli such as heat, light, pressure, solvent vapors, pH, etc. Over the past few years, there is a growing interest in developing multi-stimuli responsive fluorescent organic materials as these materials have potential applications in the field of optical sensors, chemosensors, mechanosensors, thermochromic sensors, bioimaging, data storage and security papers, etc.[1]. Phenothiazine shows a folded butterfly conformation in the electronic ground state[2]. Phenothiazine derivatives exhibit relatively intense luminescence, high photoconductivities and reversible oxidation. They also show intramolecular charge transfer (ICT) and photoinduced electron transfer (PET). These optical properties make them suitable candidates for a variety of optoelectronic applications. As a part of our research work on the synthesis of organic molecules for potential use as advanced materials[3], we have developed multi-stimuli responsive phenothiazine derivatives that display fluorochromic changes in photophysical properties in the presence of pressure, solvent vapours, heat, acid vapours, moisture etc.[4]. This recent research work from our laboratory would be discussed in greater details during the lecture.

References

1. J. Y. Zhu, C. X. Li, P. Z. Chen, Z. Ma, B. Zou, L. Y. Niu, G. Cui and Q. Z. Yang, *Mater. Chem. Front.,* 2020, **4**, 176;

   B. Roy, M. C. Reddy and P. Hazra, *Chem. Sci.*, 2018, **9**, 3592.
2. J. D. Bell, J. F. Blount, O. V. Briscoe and H. C. Freeman, *Chem. Commun.* (London), 1968, **24**, 1656.
3. H. Sharma, R. Kakkar, S. Bishnoi and M. D. Milton, *J. Photochem. Photobiol. A,* 2022, **430**, 113944;

   S. Gupta and M. D. Milton, *J. Photochem. Photobiol. A,* 2022, **424**, 113630;

   S. Gupta and M. D. Milton, *Dyes and Pigments,* 2021, **195**, 109690;

   T. Sachdeva and M. D. Milton, *J. Molecular Structure,* 2021, **1243**, 130768;

T. Sachdeva and M. D. Milton, *J. Photochem. Photobiol. A,* 2020, 112804;

T. Sachdeva and M. D. Milton, *Dyes and Pigments,* 2020, **181***,* 108539;

S. Chaudhary, M. Mukherjee, T. K. Paul, S. Taraphder and M. D. Milton, *J. Photochem. Photobiol. A,* 2020, **397**, 112509.

4. R. Kumari and M. D. Milton, *Dyes and Pigments,* 2022, **205***,* 110474;

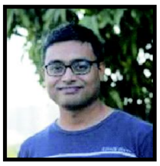
   T. Sachdeva and M. D. Milton, *Dyes and Pigments,* 2020, **181***,* 108539;

   T. Sachdeva, S. Bishnoi and M. D. Milton, *ChemistrySelect,* 2017, **2**, 11307-11313.

Brief Bio-Sketch

Prof. Marilyn Daisy Milton pursued a degree in B.Sc. Chemistry(Honours) (1995) from Miranda House, University of Delhi and M.Sc. Chemistry (1997) and Ph.D. (2002) from Indian Institute of Technology, Delhi. Later she worked as a post-doctoral researcher at Kyoto University, Japan (2002-2004) as Monbukagakusho research fellow and at Shiga University of Medical Sciences, Japan (2004-2005). She joined the Indian Institute of Technology, Kharagpur as an Assistant Professor in 2005 and worked there for two years. Later she joined the University of Delhi as a Reader in 2007, was promoted as an Associate Professor in 2008 and as Professor in 2013. Her research interests include design and synthesis of fluorescent sensors; design and synthesis of advanced materials, development of new methodologies for functional group transformations, synthesis of novel heterocyclic compounds and their applications, organocatalysis, transition-metal catalyzed cross-coupling reactions, development of multi-catalyst systems for organic transformations. She is also serving as the Editorial Board Member, Chemistry Select (2021-2025) and Member, Associate Editorial Board, Current Organic Chemistry (2019-2022).

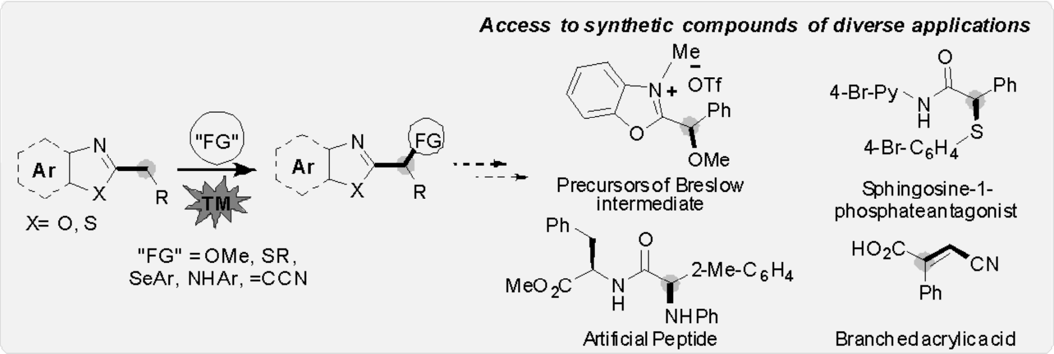
Invited Lecture-13



Catalytic functionalization of alkyl groups adjacent to azoles

Sukalyan Bhadra
Inorganic Materials and Catalysis Division,
CSIR-Central Salt & Marine Chemicals Research Institute Bhavnagar,
Bhavnagar
E-mail: sukalyanbhadra@yahoo.co.in

A plethora of bioactive compounds and natural products bear an azole subunit within their complex structural frameworks. A footstep to realize those complex structures in atom economic fashion rely on the direct functionalization of C–H bonds adjacent to an azole group. In addition, the resulting functionalized azole compounds can be simply modified into practically significant genre of α-functionalized carboxylic acids that are otherwise inaccessible through a formal α-functionalization strategy. Despite C(sp^3)–H bonds next to an azole ring are somewhat triggered by the electronic influence of the heteroaromatic system, the acidity of those C–H bonds are still low (pK_a approx. >25 in DMSO) and require a metal-catalyzed activation. We have studied the scope of functionalizing a methyl and/or methylene group(s) adjacent to an azole ring enabled by late and earth-abundant transition metals under oxidative condition. Collectively, all these new approaches have led to access otherwise challenging methoxylated (C-O)[2], chalcogenated (C-S, C-Se)[3], aminated (C-N)[4] and cyanomethylenated (=CHCN)[5] compounds in a rather simpler manner.



References

1. (a) J. Kumar, A. Rahaman, A. K. Singh and S. Bhadra, *Chem.-Asian J.*, 2020, **15**, 673;
   (b) A. Gupta, J. Kumar, A. Rahaman, A. K. Singh and S. Bhadra, *Tetrahedron,* 2021, **98**, 132415.
2. A. Gupta, A. Rahaman and S. Bhadra, *Org. Lett.*, 2019, **21**, 6164.
3. J. Kumar, A. Gupta and S. Bhadra, *Org. Biomol. Chem.*, 2019, **17**, 3314.
4. J. Kumar, E. Suresh and S. Bhadra, *J. Org. Chem.,* 2020, **85**, 13363.
5. A. K. Singh, J. Kumar and S. Bhadra, *J. Org. Chem.*, 2022, **87**, 1512.

Brief Bio-Sketch

Sukalyan Bhadra received both B.Sc. (2004) and M. Sc. (2006) degrees in Chemistry from the University of Calcutta (India). In 2011, he was awarded with a Ph.D. degree under the supervision of Professor Brindaban C. Ranu at Indian Association for the Cultivation of Science, India. He then moved to Germany, in the group of Professor Lukas J. Goossen at TU Kaiserslautern for a postdoctoral stint. Later in 2013, he joined the group of Professor Hisashi Yamamoto at Chubu University, Japan as a JSPS postdoctoral fellow. In May 2016, he returned to India as a DST-INSPIRE Faculty fellow to begin his independent career at CSIR-CSMCRI Bhavnagar, where he currently works as a Senior Scientist. His research interest revolves around development of new methodologies towards metal promoted organic transformations, α-functionalization of common building blocks, cooperative catalysis and asymmetric catalysis leading to the synthesis of fine chemicals, bioactive compounds and API molecules.

Invited Lecture-14

Redox processes in low-valent low-coordinate main-group compounds

Anukul Jana
Tata Institute of Fundamental Research Hyderabad,
Gopanpally, Hyderabad-500 046, Telangana, India
E-mail: ajana@tifrh.res.in

The synthesis of unprecedented class of compounds are always important for the development of new chemistry. Last three-four decades there has been tremendous progress in the chemistry of low-valent low-coordinate main group compounds and it is possible due to the successful isolation of this class of compounds which were once thought to be an elusive: such as singlet carbene, compounds having multiple bond between two heavier elements (e.g. disilene and diphosphene), boryl lithium, borylene and phosphinidene.

With our 7-8 years efforts we were able to developed convenient synthetic route for the syntheses of low-valent low-coordinate main-group compounds such as organic radicals[1], diradicals[2], (π-conjugated) radical-cations[3], (poly) cations[4], NHC-coordinated diphosphene/ phosphinidene/phosphinidene oxide[5], electronically/geometrically modified alkenes/imines[6] and π-conjugated molecule with electron deficient atom[7]. In my presentation I will showcase how we are employing these low-valent low-coordinate main-group compounds as a synthons and reagents by means of redox (reduction/oxidation) processes.

References

1. Mandal, *et al.*, *Chem. Sci.*, 2019, **10**, 4077-4081.
2 (a) Maiti, *et al., Angew. Chem. Int. Ed.*, 2020, **59**, 6729-6734;
   (b) Maiti, *et al., Chem. Sci.*, 2020, **11**, 11827-11833.
3. a) Mandal, *et al., Org. Lett.*, 2017, **19**, 5605-5608;
   (b) Nayak, *et al.*, *Chem. Eur. J.*, 2020, **26**, 4425-4431;
   (c) Mahata, *et al., Org. Lett.*, 2020, **22**, 8322-8336;
   (d) Mahata, *et al., J. Org. Chem.*, 2021, **86**, 10467-10473.
4. Mandal, *et al., Chem. Commun.*, 2020, **56**, 8233-8236.
5. (a) Dhara, *et al., Chem. Sci.*, 2018, **9**, 4235-4243;
   (b) Dhara, *et al., Angew. Chem. Int. Ed.*, 2019, **58**, 15367-15371;
   (c) Dhara, *et al., Chem. Commun., 2020,* **57**, 809-812;
   (d) Dhara, *et al., Chem. Commun.*, 2021, **57**, 9546-9549.

6. (a) Mandal, *et al., Chem. Eur. J.,* 2020, **26**, 5951-5955;
   (b) Anga, *et al., Eur. J. Org. Chem.*, 2020, **2020**, 7445-7449;
   (c) Nayak, *et al., Chem. Commun.*, 2021, **57**, 1210-1213;
   (d) Kundu, *et al., J. Org. Chem.*, 2021, **86**, 12683-12692.
7. Maiti, *et al., J. Am. Chem. Soc.*, 2021, **143**, 3687-3692.

Brief Bio-Sketch

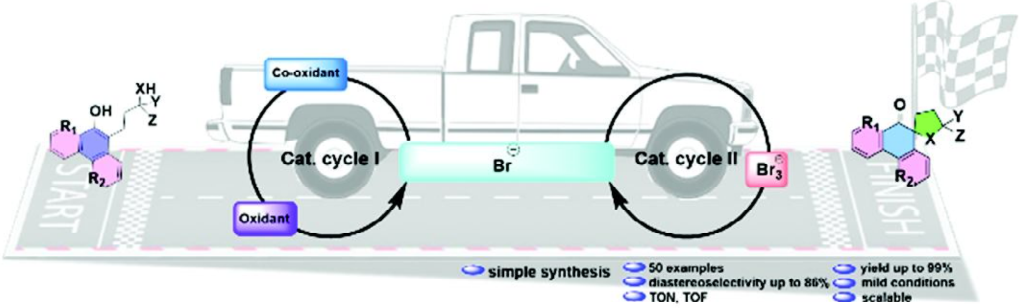
Dr. Anukul Jana obtained his Ph.D. in 2009 from University of Göttingen, Germany under the guidance of Professor Herbert W. Roesky. His doctoral thesis focused on the chemistry of compounds with low-valent Group 14 elements. He did his first post-doctoral research work as a Alexander von Humboldt fellow in the group of Professor Paul Knochel, Ludwig-Maximilians-Universität, Germany. Later on he moved to pursue his second post doctoral research in the group of Professor David Scheschkewitz, Universität des Saarlandes, Germany. In March 2014, Dr. Anukul Jana started his independent career at TIFR Hyderabad. His current research interest is mainly in the chemistry of low-valent low-coordinate Group 13-15 elements.

Invited Lecture-15

Tribromide catalysis – Newer directions of dearomative syntheses

Debayan Sarkar
Department of Chemistry,
Indian Institute of Technology Indore,
Indore
E-mail: sarkard@iiti.ac.in

In last few decades dearomative transformations has grasped immense attention of chemists and in this context, we found major reports highlighting on hypervalent iodines. **Dearomatization** of arenols is considered to be the shortest and most powerful approach towards the construction of a range of molecular architectures from simple planar starting materials. We are working on tribromide mediated dearomative *intra*- or *inter*- molecular transformations since long. This process is robust, scalable and simple. It has been a long time challenge which was now successfully been accomplished in this report, here we enlighten the tribromide catalyzed *intra*- molecular oxidative dearomative spirocyclization of arenols.



References

1. *J. Org. Chem.,* 2021, **86**, 23, 16369-16395;
   Asian Journal of Organic Chemistry, 2021, **10**, 1786-1794;
   Organic and Biomolecular Chemistry, 2020, **18**, 4619-4627;
   European Journal of Organic Chemistry, 2020, **11**, 1727-1731;
   Tetrahedron Letters , 2020 (cover page Article), **61**, 151646;

European Journal of Organic Chemistry, 2020, 397-401;
European Journal of Organic Chemistry, 2020, **7**, 891-896 ;
Organic Letters, 2019, 21, **11**, 4132-4136.

Brief Bio-Sketch

Debayan Sarkar is an associate professor of chemistry at the Indian Institute of Technology Indore, India. Before this he served NIT Rourkela as an Associate Professor. He completed his MSc with the organic chemistry specialization from the University of North Bengal (NBU) in the year 2005 followed by a PhD in organic synthesis from IACS Kolkata in the year 2011 under the supervision of Prof. R. V. Venkateswaran. After that, he travelled to carry out his post-doctoral studies at Stanford University (USA) under the mentorship of Prof. Barry M. Trost. He has also worked as visiting senior assistant professor at the Graduate School of Pharmaceutical Sciences, Tohoku University (Japan) with Prof. M. Yamaguchi and as ICMR International Research fellow at University of Regensburg Germany with Prof. Burkhard Konig. He is a recipient of prestigious awards like the DST INSPIRE Faculty Award, BRNS-DAE Young Scientist Award, Indo-US Research Award, DAAD Visiting Professor Research Award at the University of Leipzig, ICMR International Fellowship 2019 to the University of Regensburg, SERB Tetra Award and Prof. R. C. Tripathy Memorial Award for Excellence in Research, Orissa Chemical Society. His research interests include dearomatisation reactions, Visible Light catalysis, atom economic couplings and complex total synthesis of natural products. He has guided 6 Ph.D students and presently 10 Ph.D students are working in his group. He has published 56 journal papers and 1 patent.

Invited Lecture-16

Functional carbon quantum dots for chemosensing, bioimaging and therapeutic applications

Sasmita Mohapatra
Department of Chemistry,
National Institute of Technology Rourkela,
Rourkela-769 008, Odisha, India
E-mail: sasmitam@nitrkl.ac.in

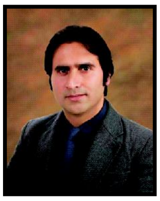
Recently carbon quantum dots (CQD) have attracted enormous interest for applications ranging from electronics, optoelectronics and photovoltaics to sensing, bioimaging, and therapeutics due to their unique physical and chemical properties. In order to broaden their applications in fluorescence sensing, especially to meet specific requirements, surface engineering, including tailoring surface functional group and subsequent chemical modification, is an effective strategy. The solution phase sensing by using CQDs can be well applied to sense various analytes, such as cations and anions, small molecules and macromolecules, cells and bacteria and so on. Apart from this, recently N-doped carbon dots with strong absorbance in the near-infrared (NIR) region are potential to act as photothermal agent. In this presentation, we will focus on our approaches to tune the responses of CQD/NCQD towards photo-interactions by choosing suitable molecular precursors in bottom up synthesis of CQD followed by subsequent surface modulations aiming at specific analytes. Also synthesis methods of some NIR-absorbing N-doped mesoporous carbon for therapeutic applications has been included in this presentation.

Brief Bio-Sketch

Sasmita Mohapatra received her Bachelor degree (B.Sc.) with honours in Chemistry from Ravenshaw College, Odisha, in 1999. She did her Masters in Chemistry from Utkal University, India in 2001. She then obtained her Ph.D. degree from Indian Institute of Technology, Kharagpur, India in 2008. Currently she is working as an Associate Professor in Department of Chemistry, National Institute of Technology, Rourkela, India. She has published 40 papers in different reputed international journals as corresponding author with a total citation of 2870 and scopus *h* index 27. She has been awarded, 1. Young Scientist Award from **State Science Academy**, Govt. of Odisha in 2014, 2. Young scientist award from **Odisha Chemical Society** in the same year. Her research is mainly directed towards the design of functional nanomaterials for sensing and medical applications.

Invited Lecture-17

Nature inspired nano/microscale janus surfaces for atmospheric water harvesting and oil/water separation



Ghulam Mohd, Kowsar Majid* and Saifullah Lone*
Department of Chemistry,
iDREAM (Interdisciplinary Division for Renewable Energy & Advanced Materials)
National Institute of Technology (NIT), Jammu & Kashmir,
Srinagar-190 006, India
E-mail: saifullah.lone@nitsri.net

The pursuit of clean and potable drinking waters is an assignment that invites collective discourse from scientists, policymakers, and innovators. In this connection, the presence of moisture in the atmosphere is considered one of the major sources of potential freshwater. Hence, fishing atmospheric water is a mammoth opportunity. Atmospheric water harvesting (by plants/or animals) in nature (particularly in deserts/ or arid regions) serves as an inspiration for crafting state-of-the-art water harvesting structures and surfaces to buffer the menace of acute water scarcity. Moreover, filtering oil/water mixtures from freshwater bodies is equally in high demand for a sustainable environment.

First, we revealed the multifunctional Janus surface traits of Trifolium Pratense (i.e., Red Clover) leaf with prominent atmospheric water fishing ability on upper and lower leaf faces. Water harvesting is performed by conical outgrowths (i.e., micro hairs). The intriguing topography of the individual hair comprises an interspersed structure for catching up air-laden moisture, merging the tiny beads of condensed water—which under gradient pull are transported to the hair base. Noticeably, instead of gravitational pull, the hairs reveal water reaping competence—under the collective impact of surface energy and Laplace pressure gradients. Consequently, both straight-up and upside-down water trapping abilities are presented. Furthermore, the leaf surface exhibits dual water wettability features. The upper front manifests the lotus effect (water-repelling with a contact angle (CA) of 156° ± 1.2° and water roll-off phenomenon at <5° SA). In contrast, the lower leaf face displays a rose petal effect (with 151° ± 2.2° CA and robust water-retaining/or pinning at 180°). The work is considered essential for a plethora of applications, including AWH, rainwater collection, self-cleaning and adhesive fixtures.

Second, we studied the Janus membrane with efficient oil-water filtration. The membrane is inspired by the lotus leaf and is crafted by the transfer printing process. The top face of the membrane is superhydrophobic, while the undersurface is hydrophilic and underwater oleophobic. A laser texturing machine is used to drill and control the size of the membrane micropores through which oil/water separation takes place. The flexible Janus membrane showed high thermal stability and ideal (i.e., 99.8%) separation. Besides having process flexibility and superior performance, the fabricated membrane is environmentally friendly and economically viable. This work could establish a scalable basis for efficient and low-cost oil/water filtration membranes to assist in building a sustainable environment.

Brief Bio-Sketch

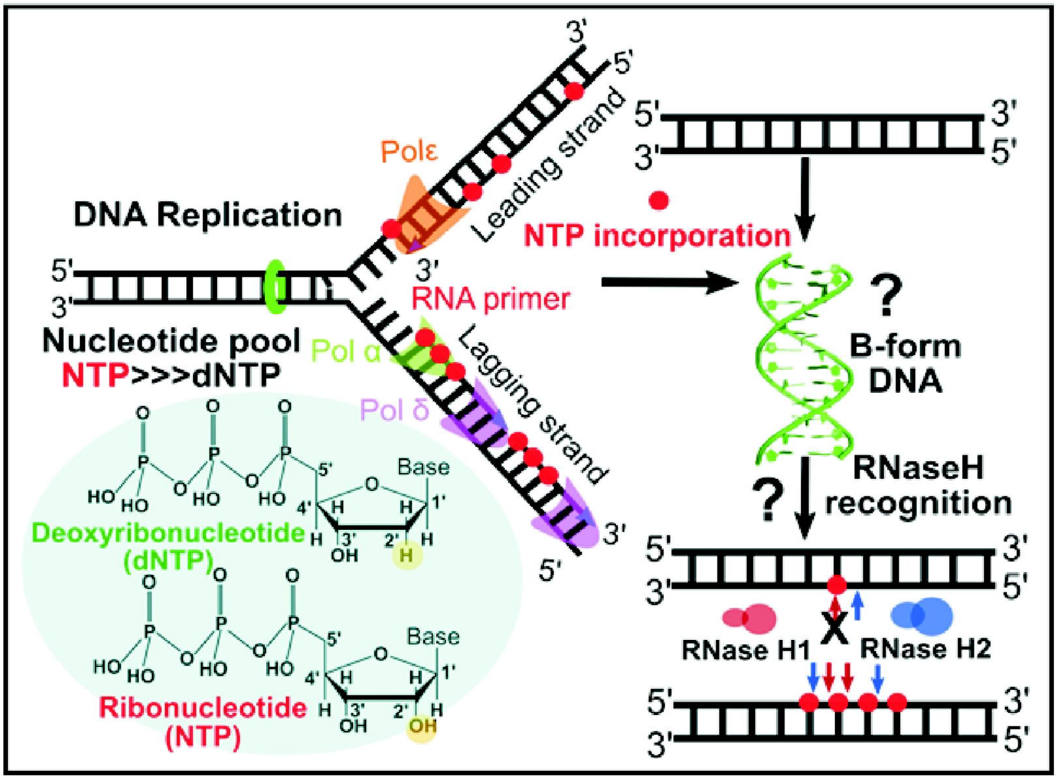
Dr. Saifullah Lone attained Bachelor's and Master's degrees in Chemistry from Aligarh Muslim University (AMU), India. He pursued Ph.D. in Droplet Microfluidics from the Department of Applied Chemistry, Kyungpook National University (KNU), South Korea, in 2012. After Ph.D. Dr. Lone worked with various universities, including—Seoul National University (SNU), King Abdullah University of Science & Technology (KAUST), Kyungpook National University (KNU), and Pusan National University (PNU) as a Foreign Researcher, Postdoctoral Fellow, and Research Professor. In 2019, Dr. Lone returned to India as Ramanujan Fellow & joined NIT Srinagar. After feeling the urgency for a quality research platform in Kashmir, Dr. Lone along with his collaborators (Particularly, Prof. Kowsar Majid - HOD Chemistry & Dr. Malik Abdul Wahid - Inspire Faculty) at NIT Srinagar established a new research center; namely, **Interdisciplinary Division for Renewable Energy & Advanced Materials (iDREAM)**. Dr. Lone is currently a Principal Investigator of **BRAINS** (**Laboratory for Bioinspired Research on Advanced Interface & Nanomaterials**) at iDREAM. His research interests are Soft Materials, Microfluidics, Soft Actuators, Solid-Liquid Interfaces, & Bioinspired Materials.

Invited Lecture-18

Conformational consequences of accommodating ribose sugars in double-stranded DNA: Insights towards protein-DNA recognition

Manjula Jaisal, Rajesh Kumar Reddy Sannapureddi,
Manish Kumar Mohanty and Bharathwaj Sathyamooorthy*
Indian Institute of Science Education and Research Bhopal,
Bhopal-462 066, Madhya Pradesh, India
E-mail: bharathwaj@iiserb.ac.in

Deoxyribose Nucleic Acids (DNA) is the predominant genetic material for living organisms, that is essentially a biopolymer composed on nucleotides containing deoxyribose sugar. Conformational flexibility of the deoxyribose sugar result in commonly observed polymorphs, i.e. A-, B- and Z-DNA, with B-DNA being the functionally relevant form in the *in vivo* conditions. On the other hand, the ribose sugar tends to favor the A-form architecture, as observed in



ribose nucleic acids (RNA). Interestingly, incorporation of ribose sugars (rNMP) in double-stranded DNA (by polymerases during replication or as primers in the Okazaki fragments) is observed to occur in the cells that alters the molecular properties of DNA. For instance, incorporating rNMP in duplex DNA the reduced compaction tendencies resulting in suboptimal genome packaging. Crystal structure studies bias the folding landscape, resulting in A-DNA formation even for the presence of one rNMP in a dodecamer DNA. NMR studies have been far and few, with minimal perturbations observed at the site of modification.

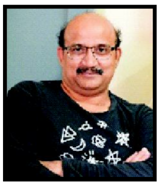
Ribonuclease (RNase) H forms a class of enzymes that recognize and repair rNMP incorporations in DNA, with RNase H1/H2 showing significant differences in their repairing of single/multiple rNMPs. Hence, we sought to study the changes in conformational properties of duplex DNA by systematically positioning single or multiple rNMP in a dodecamer sample. We performed solution-state Nuclear Magnetic Resonance (NMR) spectroscopy and molecular dynamics simulations to map the perturbations that occur at an atomistic resolution. We find characteristic changes to local structure of the modified strand and, more importantly, broadening of resonances upon ribose incorporations. In this talk, I will present the findings from this study and spotlight on how subtle changes in the chemical structure alters essential properties of this important biopolymers.

Brief Bio-Sketch

Bharathwaj secured a gold medal upon completing his bachelor's degree from the University of Madras in 2005. He pursued his Master's from IIT Madras (2007), where his interest in Nuclear Magnetic Resonance nucleated. He obtained his Ph.D. from the State University of New York at Buffalo (2013) under Prof. Thomas Szyperski, working in developing and applying solution-state NMR methodologies to study biomolecules. He then worked with Prof. Hashim Al-Hashimi (University of Michigan and Duke University, now in Columbia) in nucleic acid structure and dynamics (2013-2015). Bharathwaj has been an assistant professor at the Indian Institute of Science Education and Research (IISER) Bhopal from Dec '15 until now, leading an independent research group studying DNA and RNA conformational preferences. In particular, the lab focuses on understanding how molecular plasticity results in altered structural properties of nucleic acids.

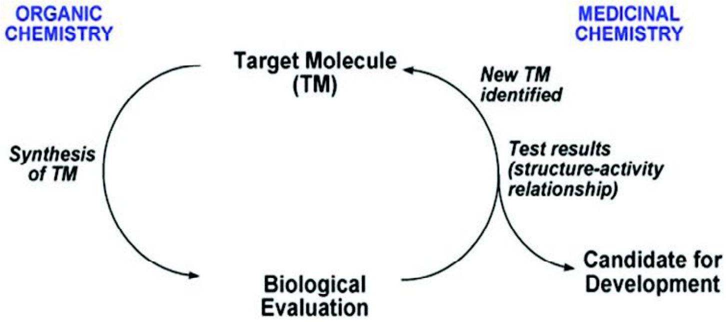
Invited Lecture-19

Expanding the medicinal chemistry toolbox: From method development to delivery of drug like molecules



Parthasarathi Das
Department of Chemistry and Chemical Biology,
Indian Institute of Technology (ISM) Dhanbad,
Dhanbad-826 004, India
E-mail: partha@iitism.ac.in

The pharmaceutical industry remains solely reliant on synthetic methodology to prepare drugs or drug like molecules for their discovery/process program. The expansion of synthetic methodology in recent years has greatly facilitated the preparation of molecules that would once have been considered an insurmountable synthetic challenge. In turn, the pharmaceutical industry, where large numbers of molecules are prepared and tested for their therapeutic use became the principal end-users and beneficiaries of this enlarged toolkit. Designing and discussing of various synthetic tools for the synthesis of pharmaceutically important heterocycles and generation of new chemotypes with translational potential will form the basic premise of my presentation[1].



References

1. (a) P. Halder, T. Roy and P. Das, *Chem. Commun.*, 2021, **57**, 5235;
   (b) S. Cardoza, M. K. Shrivash, P. Das and V. Tandon, *J. Org. Chem.*, 2021, **86**, 1330;
   (c) P. Kannaboina, K. Mondal, J. K. Laha and P. Das, *Chem. Commun.*, 2020, **56**, 11749;
   (d) K. Mondal, P. Halder, G. Gopalan, S. Sasikumar, K. V. Radhakrishnan and P. Das, *Org. Biomol. Chem.*, 2019, **17**, 5212;

(e) S. Cardoza, P. Das and V. Tandon *J. Org. Chem.*, 2019, **84**, 14015;

(f) G. Raina, P. Kannaboina, N. Mupparapu, S. Raina, Q. N. Ahmed and P. Das, *Org. Biomol. Chem.*, 2019, **17**, 2134;

(g) P. R. Nitha, M. M. Joseph, G. Gopalan, K. K. Maiti, K. V. Radhakrishnan and P. Das, *Org. Biomol. Chem.*, 2018, **16**, 6430;

(h) P. Kannaboina, G. Raina, K. Anil Kumar and P. Das, *Chem. Commun.*, 2017, **53**, 9446;

(i) P. Kannaboina, K. Anil Kumar and P. Das, *Org. Lett.*, 2016, **18**, 900.

Brief Bio-Sketch

Parthasarathi Das received his Ph D degree from **CSIR-National Chemical laboratory**, Pune, India in 1999. He did post-doctoral studies (1999-2003) at the **RWTH-Aachen, Germany**, **Tohoku University**, Japan and **Harvard University**, USA. In 2003 he moved to India to join Discovery Research of **Dr. Reddy's Laboratories Ltd.** and worked in medicinal chemistry group having research focus on various therapeutic areas e.g., oncology, metabolic disorder and antibacterial. After completing ten years in Industry, in 2012 he moved to academia and joined **CSIR-Indian Institute of Integrative Medicine**, Jammu. In 2017 he moved to **Indian Institute of Technology (ISM) Dhanbad** and joined as faculty in the Department of Chemistry and Chemical Biology. His current research interests include medicinal chemistry, development of new synthetic tool and synthesis of biologically active natural products. He has been selected for **Chemical Research Society of India (CRSI) Bronze Medal**, 2019 for his contribution to research in chemistry. He is a Fellow of the Royal Society of Chemistry (**FRSC**) and at present he is the **Head of Department of Chemistry and Chemical Biology**, IIT (ISM) Dhanbad.

Invited Lecture-20

Dynamics of H_2O dissociation on metal surfaces

Ashwani K. Tiwari
Department of Chemical Sciences,
Indian Institute of Science Education and Research Kolkata,
Mohanpur-741 246
E-mail: ashwani@iiserkol.ac.in

Dissociation of H_2O on a metal surface is rate-limiting step in many industrially important reactions. In a few recent experiments, it has been observed that dissociation of H_2O on a metal surface is mode-selective. In other words, this reaction is not statistical in nature and therefore, one cannot use transition state-based theories to get insights of this reaction. Our quantum dynamical calculations show that mode-mode coupling along the reaction path is the key factor in deciding the quantum of mode-selectivity in this reaction.

Brief Bio-Sketch

Ashwani K. Tiwari received his Ph.D. in 2007 from the Indian Institute of Technology Kanpur under the supervision of Prof. N. Sathyamurthy. During the period from May 2007 to April 2008, he was a postdoctoral researcher with Prof. Niels E. Henriksen at the Technical University of Denmark. From May 2008 to April 2010, he was a postdoctoral fellow with Prof. Bret Jackson at the University of Massachusetts, Amherst. He joined the Indian Institute of Science Education and Research Kolkata as an assistant professor in October 2010, and now he is a professor at the same institute. His research interests involve the dynamics of laser-molecule and molecule-metal surface interactions. Recently, he received the Chemical Research Society of India (CRSI) Bronze Medal and was elected as a fellow of Royal Society of Chemistry.

Invited Lecture-21

Identification of Rottlerin as a broad-spectrum antiviral against multiple RNA viruses

Durbadal Ojha and Karin E. Peterson
Rocky Mountain Laboratories,
National Institute of Allergy and Infectious Diseases,
National Institutes of Health, Hamilton, MT, USA
E-mail: durbadal.ojha@nih.gov

The primary treatment for viral encephalitis is palliative care due to the lack of therapeutics. We conducted a screen of 3,833 FDA approved and bioactive small molecules against La Crosse virus (LACV), a mosquito borne Orthobunyavirus that is a leading cause of pediatric arboviral encephalitis in the United States. We found one compound, Rottlerin (RTL), which inhibited LACV-induced apoptosis in human and murine neuronal cell lines as well as human cerebral organoids. Mechanistic study showed that RTL treatment inhibit virus replication by preventing trafficking from the Golgi apparatus. *In vivo*, RTL significantly inhibited LACV-induced disease in a mouse model, even though administration of the drug was delayed until 3 days post-infection, a time point when virus is already detected in the central nervous system. Analysis of other RNA viruses showed that RTL could inhibit Zika virus and SARS-CoV-2 virus replication. Indeed, RTL treatment significantly reduced SARS-CoV-2-induced mortality in Human ACE2 expressing K18 mice by approximately 40%. Collectively, these studies indicate that RTL is an effective broad-spectrum antiviral particularly in the context of emerging RNA viruses infections.

Brief Bio-Sketch

Dr. Durbadal Ojha was awarded his Ph.D. (2016) in Virology from Jadavpur University and Indian Council of Medical Research Virus Unit, Kolkata, India. He specialized in analyzing anti-viral properties of traditional medicines and ethnomedicinal plants. He is currently a post-doctoral fellow in the Neuroimmunology Section, studying drug development against different types of RNA viruses.

Invited Lecture-22

Unique carbon nanodots derived from waste plastic and their solar energy harvesting applications

Ujjal K. Gautam
Department of Chemical Sciences,
Indian Institute of Science Education and Research, Mohali,
Punjab
E-mail: ujjalgautam@gmail.com
ujjalgautam@iisermohali.ac.in

The reduction of plastic-waste has emerged as a research priority, leading to many innovative approaches to convert them into useful materials. In this talk, I will describe a rational strategy for converting waste plastic into photocatalytic carbon quantum dots (CQDs) in a residue-free, inexpensive and impurity-free manner. I will further discuss a unique property that the CQDs exhibit an ability to harvest molecular oxygen from the air, thereby resulting in ultrahigh photocatalytic oxidation efficiency in chemical transformations under ambient conditions and natural sunlight. It was further found that the amount of oxygen adsorbed on the CQD surfaces are different in the dark and under light illumination. The excitons generated under light induce desorption of the O_2 molecules, a phenomenon that we have named as 'light-induced hypoxia'. We further demonstrated that when not performing any reaction, the CQDs exhibit self-sensitized pho-oxidation and produce CO_2, thus removing themselves from the reaction media. This is a new material property that we term as 'CQD-autophagy' and beneficial as removal of photocatalysts is an expensive process in industrial-scale applications.

Brief Bio-Sketch

Dr. Ujjal K. Gautam completed his master's studies in Chemistry from IIT D in 1999 and Ph.D. from the SSCU, IISc in 2006 under the supervision of Prof. C. N. R. Rao, FRS.

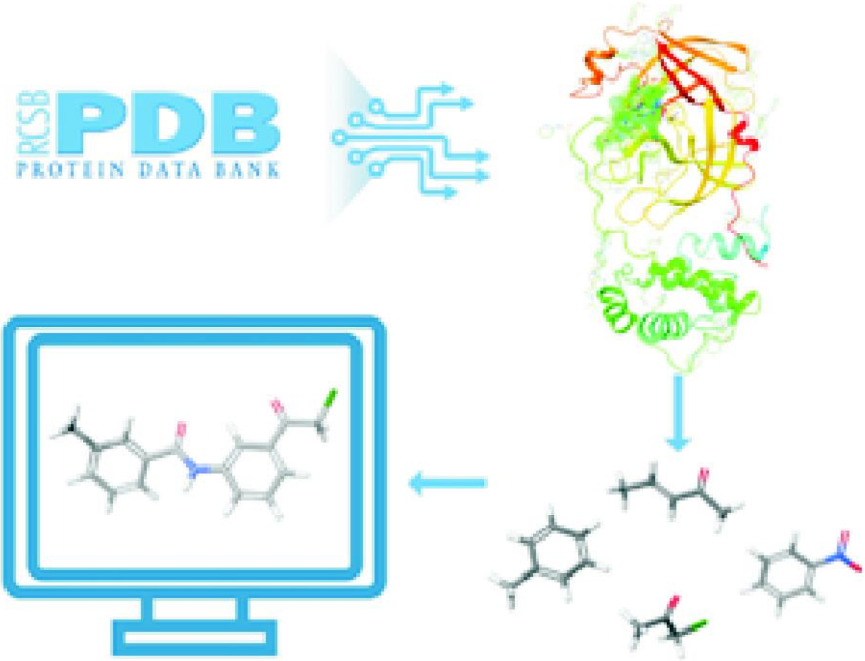
Thereafter, he was a postdoctoral researcher at NIMS, Tsukuba, Japan for two years before joining a tenure track ICYS independent researcher position at the same institution. Dr. Gautam joined JNCASR in 2011 as a Ramanujan Fellow and worked until 2016. In 2016, he joined IISER Mohali as an Assistant Professor. His research interest revolves around developing high-quality nanostructured materials for renewable energy harvesting and environmental remediation. He has published over 100 papers in high-quality peer-reviewed journals and also owns about 8 patents to his name.

Invited Lecture-23

Non-covalent interaction based drug designing

Nayim Sepay
Department of Chemistry,
Lady Brabourne College,
Kolkata-700 017, India
E-mail: nayimsepay@yahoo.com

Drug designing is the innovative method to find new compounds based on the knowledge of a biological target. The research field is divided into two major two classes 1. Structure-based drug designing and 2. Ligand-based drug designing. In the first case, the structure of a protein is used as the basis to identify or design new chemical compounds that could bind to the target resulting in inhibition of the target protein[1]. Again, ligand based drug design is an approach used in the absence of the receptor 3D information and it relies on knowledge of molecules that bind to the biological target of interest[2]. This work represents a new class of drug designing. In this method large number of protein molecules are used to get a knowledge of noncovalent interactions distributed in the active site of the protein. In this way, important amino acids, types of interactions and functional groups in small molecules are



required for good interaction can be identified. This knowledge was used to design new pharmacophore or lead molecule[3,4].

References

1. M. Batool, B. Ahmad and S. Choi, *Int. J. Mol. Sci.*, 2019, **20**, 2783.
2. P. Aparoy, K. Kumar Reddy and P. Reddanna, *Curr. Med. Chem.*, 2012, **19**, 3763-3778.
3. N. Sepay, P. C. Saha, Z. Shahzadi, A. Chakraborty and U. C. Halder, *Phys. Chem. Chem. Phys.*, 2021, **23**, 7261-7270.
4. N. Sepay, M. Banerjee, R. Islam, S. P. Dey and U. C. Halder, *Phys. Chem. Chem. Phys.*, 2022, **24**, 6605-6615.

Brief Bio-Sketch

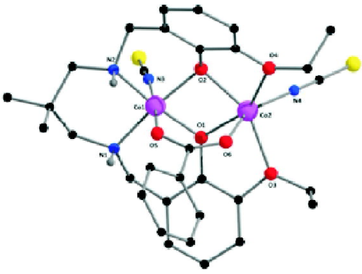
Dr. Nayim Sepay, serving as Teacher and Researcher in the Department of Chemistry (UG and PG), Lady Brabourne College, Kolkata. He studied Chemistry at New Alipore College (in UG course) and Ramakrishna Mission Vivekananda Centenary College (in PG course). He Joined Jadavpur University in 2017 for Ph.D. in science degree under Professor Asok Kumar Mallik. He developed various green methods for the synthesis of organic bio-inspired molecules. After his Ph.D., he joined Professor Umesh Chandra Halder in the same department of the university and worked on protein chemistry and related theoretical chemistry. He acted as a resource person in PG courses of Chemistry at Diamond Harbour Women's University and JIS University for teaching various parts of chemistry including Green Chemistry, and Medicinal Chemistry. He has been working as a guest faculty of Chemistry at Jadavpur University. Dr. Sepay has published 80 research papers and one textbook on Green Chemistry. As an independent researcher, his current research area focused on MOLECULAR ENGINEERING with the help of non-covalent interactions. It is based on designing and synthesis novel materials and investigating how their properties connect with their molecular structures. He studies non-covalent interactions to understand the properties of the molecules, their mechanism of action during interactions with biomacromolecules and their self-assembly.

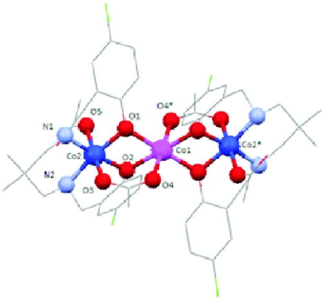
Invited Lecture-24

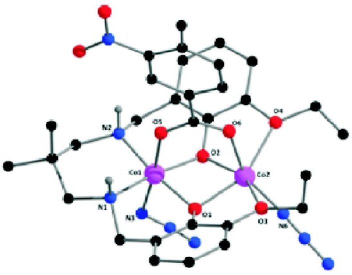
Synthetic strategies, structures and properties of cobalt(III/II) complexes with salen type Schiff bases and their reduced analogous

Shouvik Chattopadhyay
Department of
Jadavpur University
Kolkata-700 032, India
E-mail: shouvik.chem@gmail.com

A variety of polynuclear cobalt complexes with H_2 salen type Schiff bases and their reduced analogues have been synthesized in our laboratory. The complexes have been characterized by spectroscopic measurements and their solid state structures have been determined by single crystal X-ray diffraction analysis. The properties and applications of the complexes were also explored. In this talk, I shall represent an overview on the synthetic strategies, structures, and properties of these complexes. The complexes may grossly be divided into three major sub classes; Cobalt(II), cobalt(III) and mixed valence cobalt(III)/cobalt(II) complexes. Different synthetic strategies have been applied for their preparation. In most of the cases, mixed valence complexes have been synthesized by the *in situ* partial (aerial) oxidation of cobalt(II) to cobalt(III). Structures and application of the complexes will also be discussed in brief.







Brief Bio-Sketch

Prof. Shouvik Chattopadhyay did his M.Sc from the University of Calcutta in the year 2003 and obtained Ph.D (2008) from the University of Calcutta under the supervision of Prof. Ashutosh Ghosh. Presently, he is a Professor, Department of Chemistry, Jadavpur University, Kolkata. Prof.

Chattopadhyay is the Life Members of Indian Chemical Society, Indian Science Congress Association and Chemical Research Society of India. He has published more than 215 papers in reputed International Journals and supervised Ph.D thesis of 15 students. Presently, 10 Ph.D students are working under his supervision. The research interests of Prof. Chattopadhyay are Synthesis and characterization of transition and non-transition metal complexes and exploration of their catalytic, magnetic, opto-electronic and luminescence properties.

Invited Lecture-25

Demystifying the mystery of protein misfoldings in neurodegenerative diseases

Krishnananda Chattopadhyay
Structural Biology and Bioinformatics,
CSIR-Indian Institute of Chemical Biology,
Kolkata-700 032, India
E-mail: krish@iicb.res.in

Protein aggregation and deposition has been found to be a common phenotype in multiple neurodegenerative diseases. The heterogeneity of aggregation process and the presence of large number of triggering mechanisms results in the difficulty to devise therapeutic strategies against these toxic inclusions formation. Our laboratory has been investigating these triggers, which contribute to the alteration of folding pathways leading to the early and unexplored stages of aggregation. The conformational heterogeneity of the early intermediates and their transient nature are some of the reasons why traditional techniques do not typically work for the early stage detection. We have been using sensitive biophysical methods to directly detect and characterize the early intermediates and oligomers *in vitro* and inside live cells using Parkinson's diseases (PD) and ALS as our models. We are also using cryo-EM to investigate the structural insights into the early intermediates, which are believed to the primary inducer of cellular toxicity. Using a combination of biophysics, biochemistry and microscopy, we are developing protein early intermediates vs toxicity maps to determine the structural insights responsible for the neuronal toxicity.

Brief Bio-Sketch

Krishnananda Chattopadhyay is currently a Senior Principal Scientist and the Head of the Structural Biology and Bioinformatics Division at CSIR-Indian Institute of Chemical Biology. His research group applies novel biochemical and biophysical tools at ensemble and single molecule resolution to study human diseases with particular emphasis to neurodegeneration and infections.

Krishnananda Chattopadhyay obtained his PhD degree from Tata Institute of Fundamental Research, Mumbai. He then moved to Washington University School of Medicine, Saint Louis, USA for his postdoctoral research. Before joining CSIR-Indian Institute of Chemical Biology in 2006, he worked at Pfizer, USA as a Senior Scientist. He is a fellow of Royal Society of Chemistry and West Bengal Academy of Science and Technology. He is also a fellow of Indo-US Science and Technology Forum and a recipient of American Chemical Society Membership Award.

Contributory Section

[1 – 165]

Contributory Paper-1

Photochemical [2+2]-cycloaddition reaction in coordination polymers: Exploration of potential applications

Basudeb Dutta*
Department of Chemical Sciences,
Indian Institute of Science Education and Research Kolkata,
Mohanpur-741 246, West Bengal, India
E-mail: dutta.basu11@gmail.com

The exploration on metal and organic ligand composed coordination polymers (CPs) has been incipient at an astonishing pace from its existence. The promising applications and essential diversity in structure of these materials are the driving force behind the extensive research of such kind. Actually, inorganic metal ions and organic ligands (carboxylate, sulphate etc.) or neutral donor molecules (N, S donor's based pyridyl and thiophen etc.) are contented to formulate these polymeric coordination compounds. This is the leading accessories to the advancement of solid-state coordination chemistry which is termed as 'crystal engineering' presented by Schmidt. Although, this terminology has been used in regard to the solid-state photochemical [2+2] cycloaddition reaction for first time. Subsequently, this [2+2] cycloaddition reactions have been unveiled within the CP systems and resulting structural transformation promotes different potential applications: gas sorption, magnetism, sensing, dielectric property, isolation of new organic ligand, electrical conductivity, photo salient effect, flexibility and elasticity of materials. Therefore, here we are searching out the contribution of [2+2] cycloaddition reaction of CPs for the impact of different applications.

Contributory Paper-2

Green additives used as pour point depressant for Indian waxy Crude Oil

Biswadeep Pal and Tarun Kumar Naiya*
Department of Petroleum Engineering,
Indian Institute of Technology
(Indian school of mines), Dhanbad
*E-mail: tarunnaiya@iitism.ac.in

Objectives/Scope:

Crude oil production from conventional and unconventional reservoirs in colder temperature create problems of upstream industries. Wax deposited in pipeline which led critical challenges of flow assurance problems during production and transportation operations.

Mechanical, thermal and chemical methods are three general methods available in oil industry. Chemical methods are most economic process to break the wax interlocking structure for reducing the viscosity and pour point of crude oil.

Methods, Procedures, Process:

Long fatty acid based oleate ester (LOE) was synthesized from oleic acid which was separated from olive oil followed by trans-esterification reaction was conducted under N_2 environment. Theoretical amount of water was separated from dean stark apparatus.

Crude oil sample was prepared by removing water by dean stark apparatus otherwise it gives us error in result. SARA analysis was done with the help of fan *et al.* (2002). Pour point, water content and API gravity were measured by ASTM standard procedure.

Results, Observations, Conclusions:

Pour point was measured by ASTM D5853 procedure with and without LOE. It was found that after treating crude oil with 800 ppm LOE the pour point was reduced 9°C. Rheological studies were found that 63% reduction of viscosity was observed after treating with 800 ppm LOE.

Novel/Additive Information:

The synthesized LOE was prepared from vegetable oil and due to bio-degradability it is safe to use in any condition.

Contributory Paper-3

Synthesis, characterization and *in-vitro* antimicrobial activity of divalent cobalt complexes of 3-{[(4,6-dihydroxy pyrimidin-2-yl)imino]methyl} napthalen-2-ol

D. T. Sakhare
U.G, P.G. & Research Centre, Department of Chemistry,
Shivaji Arts, Comm. & Science College Kannad,
Aurangabad-431 103, Maharashtra, India
E-mail: sakharedhondiram@yahoo.com

In this work, heterocyclic Schiff bases ligands derived from 2-amino-4,6-dihydroxypyrimidine with 2-hydroxy-1-naphthaldehyde (L_1) was synthesized. These ligand used to synthesis complexes of Ni(II). The synthesized compounds have been characterized by FT-IR, ^{1}H-NMR and UV-Vis techniques for the ligands and FT-IR, UV-Vis, all reactions monitored by TLC, molar conductivity and magnetic susceptibility measurements for the corresponding complexes. General formula of complexes are $[Co(L_1)_2(H_2O)_2]$. The complexe is paramagnetic. The results of the molar conductivity measurements indicated that all complexes are non-electrolytes in (DMSO). An octahedral geometry for all the complexes of the ligands are bidentate, (L_1) through phenolic (OH) and azomethine nitrogen. The ligand and its complexes were screened for their antifungal and antibacterial activity against *Aspergillus niger, Penicillium chrysogenum, Fusarium moneliforme* and *Aspergllus flavus* and *Escherichia coli, Salmonella typhi, Staphylococcus aureus, B. subtilis.* The result indicated that the complexes exhibited good antifungal and antibacterial activities.

References

1. D. T. Sakhare, Synthesis, characterization and biological studies of aminopyrimidine Schiff bases and their transition metal complexes, *Dickensian Journal*, 2022, **22(4)**, 65-77.
2. D. T. Sakhare, Synthesis, characterization and antimicrobial activities of some Mn(II) and Fe(III) complexes of biologically active bidentate ligands, *Journal of Chemical and Pharmaceutical Research*, 2015, **7(6)**, 198-204.
3. C. Chandramouli, M. R. Shivanand, T. B. Nayanbhai, B. Bheemachari and R. H. Udupi, Synthesis and biological screening of certain new triazole Schiff bases and their derivatives bearing substituted benzothiazole moiety, *J. Chem. Pharm. Res.*, 2012, **4**, 1151-1159.
4. D. T. Sakhare, Syntheses, characterization of some transition metal complexes of bidentate Schiff base and their antimicrobial activities, *Der Chemica Sinica*, 2015, **6(6)**, 1-6.
5. V. Sharma, N. Chitranshi and A. K. Agarwa, Significance and biological importance of pyrimidine in the microbial world, *Inter. J. Med. Chem.*, 2014, 1-31.

Contributory Paper-4

2,4,6-tri(thiophen-2-yl)-1,3,5-triazine based porous polymers with nitrogen rich moieties: Synthesis and gas selectivity study

Neha Rani Kumar[a], Prasenjit Das[b], Abhijeet R. Agrawal[c],
Sanjay Kumar Mandal*[b] and Sanjio S. Zade*[c]
[a]Department of Chemistry,
Dhemaji College, Dibrugarh University,
Dhemaji-787 057, Assam, India
[b]Department of Chemical Sciences,
Indian Institute of Science Education and Research (IISER) Mohali,
Manauli-140 306, Punjab, India
[c]Department of Chemical Sciences,
Indian Institute of Science Education and Research (IISER) Kolkata,
Mohanpur-741 246, West Bengal, India
E-mail: nehakumar0926@gmail.com

Here we report an inexpensive $FeCl_3$ mediated polymerization method to synthesize triazine-carbazole based polymers by oxidative polymerization and Friedel Crafts polymerization. The synthesis of theinyltriazine and carbazole based porous polymer has been achieved under a variety of reaction conditions in the presence of $FeCl_3$ and we have shown the effect of reaction condition on the porous property of the polymer. The cross-linked flexible polymers display high thermal stability and CO_2 uptake reaching as high as 16.5 wt% at 263 K and 1 atm. The polymers also display high CO_2 selectivity over nitrogen. These polymers can be potential materials for further exploration in reactions involving the CO_2 trapping and conversion. Preliminary investigation also suggests the ability of these polymers to be used in purification purposes. These materials hold the potential as organic semiconductors for energy and environmental applications.

References

1. Y. Yuan, H. Huang, L. Chen and Y. Chen, *Macromolecules*, 2017, **50**, 4993-5003.
2. Q. Chen, M. Luo, P. Hammershoj, D. Zhou, Y. Han, B. W. Laursen, C. G. Yan and B. H. Han, *J. Am. Chem. Soc.*, 2012, **134**, 6084-6087.

Contributory Paper-5

Molecular insight into the high thermal stability of metalloprotein azurin

A. Joy[a] and R. Biswas[b]
[a]Department of Chemistry,
Indian Institute of Technology Tirupati,
Yerpedu-517 619, Andhra Pradesh, India
[b]Department of Chemistry and Center for Atomic,
Molecular and Optical Sciences & Technologies,
Indian Institute of Technology Tirupati,
Yerpedu-517 619, Andhra Pradesh, India
E-mail: rajib@iittp.ac.in

We investigate the events characterising the steps of the unfolding pathway of blue copper metallo protein Azurin using replica exchange molecular dynamics (REMD). Our studies show that the unfolding of Azurin begins with the melting of α-helix and β-sheets II and V. This is followed by the melting of other β-sheets, and the hydrophobic protein core exposes to the solvent resulting in disruptions of its tertiary structure. We constructed free energy surfaces at different temperatures which portray different basins, and signify the stability of different melted structures in the unfolding process. The contact maps at different temperatures reveal that, the strong hydrophobic interaction within the core of the protein is the vital force that renders high stability to this protein. Analysis of the individual β-sheets by looking into their amino acid sequence points out that β-sheets with charged side chains on the surface are melted fast compared to others. The β-barrel of Azurin is able to dynamically rearrange, and it helps the protein to preserve its hydrophobic core holding back the native topology from melting fast. B-factor analysis shows that residues of β-sheets III, IV, and VII are less deviating from their initial structure at the transition temperature.

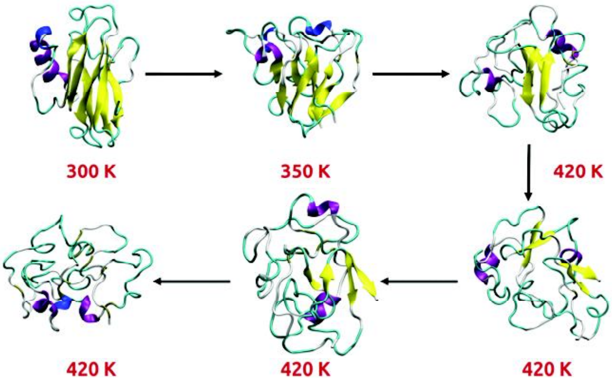


Fig. 1. The schematic representation of the melting process of azurin taken from different basins on the free energy surfaces. The α-helix is first melting secondary element followed by β-sheet V and II.

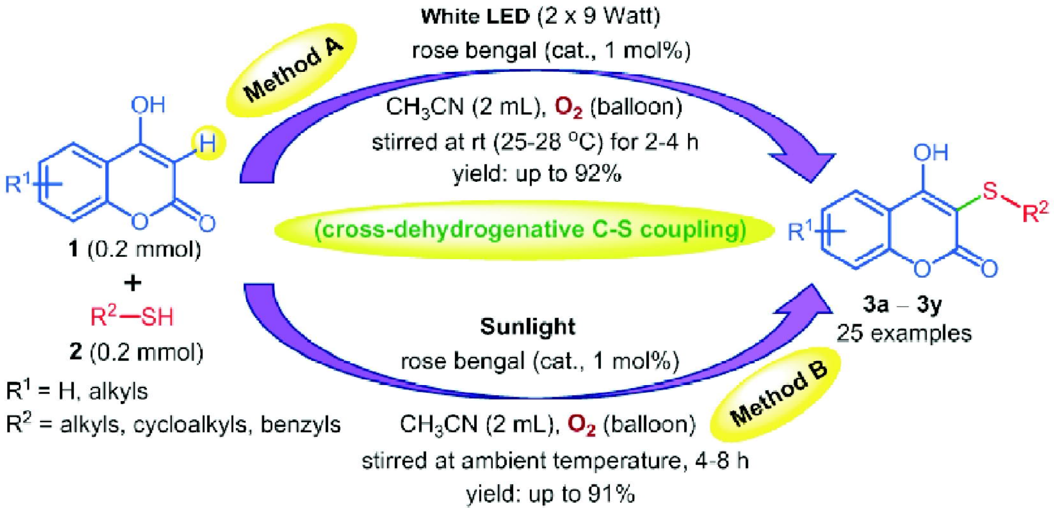
Contributory Paper-6

Visible light-promoted *cross*-dehydrogenative C3–H sulfenylation of 4-hydroxycoumarins with thiols using Rose Bengal as a photosensitizer

Anindita Bhowmick and Goutam Brahmachari*
Laboratory of Natural Products & Organic Synthesis,
Department of Chemistry, Visva-Bharati (a Central University),
Santiniketan-731 235, West Bengal, India
*E-mail: brahmg2001@yahoo.co.in
goutam.brahmachari@visva-bharati.ac.in

In recent times, the direct C–H bond functionalization, categorically, the cross-dehydrogenative coupling (CDC) reaction between two C–H/C–H and X–H (X = heteroatom) centres has become the choice of C–H functionalization for diverse molecular scaffolds due to its many inherent advantages. Among such *cross*-dehydrogenative C–X coupling reactions, forming a C–S bond is of practical utility and fundamentally challenging in modern organic synthesis. In resonance with these facts coupled with the upsurge in green chemistry practice, visible-light-induced *cross*-dehydrogenative C–S coupling is currently gaining prior attention to the organic chemists to overcome undesired synthetic issues far as practicable.

Organosulfur compounds are potentially useful and play a vital role in numerous bioactive natural products, pharmaceutical and medicinal entities, agrochemicals, and valuable materials with multifaceted uses. As part of our ongoing endeavours in green chemistry-directed organic synthesis, we recently developed a visible-light-driven green and efficient method to synthesize a new series of functionalized 3-(alkyl/benzylthio)-4-hydroxy-2*H*-chromen-2-ones **3** through *cross*-dehydrogenative C3-H sulfenylation of 4-hydroxycoumarins **1** with thiols **2**, using either white LED or direct sunlight as a visible-light energy source and rose bengal as a triplet photosensitizer for molecular oxygen (O_2) at ambient temperature (Scheme 1). The salient features of this present protocol are mild reaction conditions, energy efficiency, metal-free synthesis, use of low-cost substrates and non-toxic photocatalyst, good yields and high atom-economy, and eco-friendliness. The use of abundant sunlight offers an added advantage to this methodology.



Scheme 1

Related literature

1. M. Mandal and G. Brahmachari, *J. Org. Chem.*, 2022, **87**, 4777-4787.
2. I. Karmakar and G. Brahmachari, *Green Chem.,* 2022, **24**, 2825-2838.
3. G. Brahmachari, A. Bhowmick and I. Karmakar, *J. Org. Chem.*, 2021, **86**, 9658-9669.
4. G. Brahmachari, *et al., Green Chem.*, 2021, **23**, 4762-4770.
5. G. Brahmachari and I. Karmakar, *J. Org. Chem.*, 2020, **85**, 8851-8864.
6. G. Brahmachari, *Adv. Synth. Catal.*, 2020, **362**, 5411-5421.
7. G. Brahmachari, *et al., J. Org. Chem.*, 2020, **85**, 8405-8414.

Contributory Paper-7

Inhibition of lactate dehydrogenase A (LDH-A) by diclofenac sodium induces apoptosis in cervical cancer cells by activation of AMPK

Avirup Malla[a,b], Runa Sur[a] and Suvroma Gupta[b]
[a]Department of Biophysics,
Molecular Biology and Bioinformatics,
University of Calcutta, India
[b]Department of Biotechnology,
Haldia Institute of Technology, India
E-mail: avirupmalla@gmail.com

Warburg effect is one of the major hallmarks of cancer where a cancer cell prefers to choose glycolytic pathway over entering into oxidative phosphorylation. This metabolic switch produces instant energy required for maintaining the tumour microenvironment and performing many cellular functions. Lactate dehydrogenase A (LDH-A) is a key enzyme that facilitates glycolysis by converting pyruvate to lactate and has been shown to be upregulated in multiple cancers and is associated with tumour progression. Thus LDH-A remains a major target for various novel anticancer agents. Diclofenac (DCF) is a non-steroidal anti-inflammatory drug (NSAID) which has long been used as a common painkiller (Voltaren) for its anti-inflammatory activities. A few reports suggest that DCF has anti-cancer properties in many cancer cells lines mainly by inhibiting glucose uptake or by inhibiting glucose transporter in the cell. We have found that DCF treatment renders cytotoxic effects on cervical cancer cells. Further our results using in silico, biochemical and biophysical studies reveal that DCF dose dependently inhibits LDH-A activity in cells without effecting its expression. DCF was found to decrease lactate, NAD^+ and ATP production in cells and this could a possible mechanism by which DCF inhibits glucose uptake in cancer cells. We have additionally shown that this lowering in ATP levels in turn activates AMPK (AMP activated protein kinase), a sensor kinase which in turn leading to mitochondria mediated apoptosis. Thus, for the first time we report a NSAID group drug as an LDH-A inhibitor as well as AMPK activator. DCF or its various derivatives could serve as lead compounds for the development of targeted antimitotic compounds used for inhibiting cancer metabolism.

Contributory Paper-8

Copper(II)-Chloro-triphenylphosphine-arylazoimidazole complexes: Synthesis, Spectroscopic and redox study

Prithwiraj Byabartta
Department of Chemistry,
Jogesh Chandra Chaudhuri College,
30, Prince Anwar Shah Road,
Kolkata-700 033
E-mail: prbjccc@gmail.com

Running years have witnessed a great deal of interest in the synthesis of the complexes of gold with α-diimine type of ligands because of their photochemical, catalytic properties[2,6,16], energy conversion and ability to serve as building blocks in supramolecular arrays. Today *in vivo* biochemistry of gold remains enigmatic, mainly due to a paucity of adequate models and an inadequate understanding of the reactivity of copper. Moreover, as copper is not a metal naturally used in metabolism, it is believed that its chemistry *in vivo* differs from other transition metals such as iron and copper, which are carefully transported and stored by enzymatic processes. The biochemistry of copper with D-penicillamine, gluthadione, thiomalic acid 2,3-dimercaptopropanol, and albumin has been studied. [Ag(tht)(OTf)] assisted reaction produce $[Cu^{II}(PPh_3)Cl(tht)_2](OSO_2CF_3)_2$, reacts with RaaiR$^{/}$ in dichloromethane medium followed ligand addition leads to $[Cu^{II}(PPh_3)Cl(RaaiR^{/})](OTf)_2$ [RaaiR$^{/}$ = *p*-R-C_6H_4-N=N-C_3H_2-NN-1-R$^{/}$,(*1-3*), abbreviated as N,N$^{/}$-chelator, where N(imidazole) and N(azo) represent N and N$^{/}$, respectively; R = H (*a*), Me (*b*), Cl (*c*) and R$^{/}$ = Me (*1*), CH_2CH_3 (*2*), CH_2Ph (*3*), PPh_3 is triphenylphosphine, OSO_2CF_3 is the triflate anion, tht is tetrahydrothiophen]. The maximum molecular peak of the corresponding molecule is observed in the ESI mass spectrum. Ir spectra of the complexes show -C=N- and -N=N- stretching near at 1590 and 1370 cm^{-1} and near at 1100, 755, 695, 545, and 505 cm^{-1} due to the presence of triphenylphosphine. The ^1H NMR spectral measurements suggest methylene, $-CH_2-$, in RaaiEt gives a complex AB type multiplet with coupling constant of av. 6 Hz while in RaaiCH$_2$Ph it shows AB type quartets with coupling constant of av. 5 Hz. ^{13}C (H)NMR spectrum suggest the molecular skeleton. In the ^1H-^1H COSY spectrum as well as contour peaks in the ^1H-^{13}C HMQC spectrum assign the solution structure. Electrochemistry assign ligand reduction.

Contributory Paper-9

Liquid-liquid interface as a scaffold for fabrication of nanoparticle decorated superstructures and devices

Mohammed Ali[a] and Sujit Kumar Ghosh[b]
[a]Department of Chemistry,
Hatsingimari College, Hatsingimari,
Assam-783 135, India
[b]Department of Chemistry,
Assam University, Silchar,
Assam-788 011, India
E-mail: mali7652@gmail.com
sujitkchem.aus@gmail.com

Liquid-liquid interface is the junction of two immiscible liquids, it is a heterogeneous system involving two solvents of different solvation characteristics. The interface between two immiscible liquids is a unique environment, where, the structural, dielectric, dynamic, thermodynamic, adsorption-desorption and other surface properties and even chemical environments are also different from those of the bulk liquids. Processes occurring at this interface underlie many important phenomena in chemistry and biology. About a century ago Pickering discovered that colloidal solid particles could get adsorbed into the liquid-liquid interface which is driven by the reduction in interfacial energy. Functionalized nanoparticles are ideal candidates for technological applications of interfacial self assembly process, as they posses tunable properties and moreover the ligand attached to the nanoparticle surface can be tuned to tailor interparticle interactions. The unique physical and chemical environment at the liquid-liquid interface has been exploited in designing nanoparticle decorated devices, which includes fabrication of nanoparticle-decorated membranes, micro-capsules, raspberry-like hollow spheres, giant supramolecular assemblies and nanorods by oriented attachment of primarily formed nanospheres at different aqueous-organic interfaces. Varieties of ligand cross-linking strategies, such as, ion-pair formation, diazo reaction, polymerization and click reaction have been adopted in order to impart mechanical strength and robustness to the as-synthesized assemblies. The assemblies so obtained have been characterized by transmission electron microscopy, scanning electron microscopy, atomic force microscopy, optical and fluorescence microscopy, absorption, fluorescence and Raman spectroscopy, energy dispersive X-ray analysis, Fourier transform infrared spectroscopy, X-ray diffraction and thermogravimetric analysis. Application of these nanoparticle-decorated superstructures has been envisaged in catalysis, electrochemical sensing and ultra-filtration.

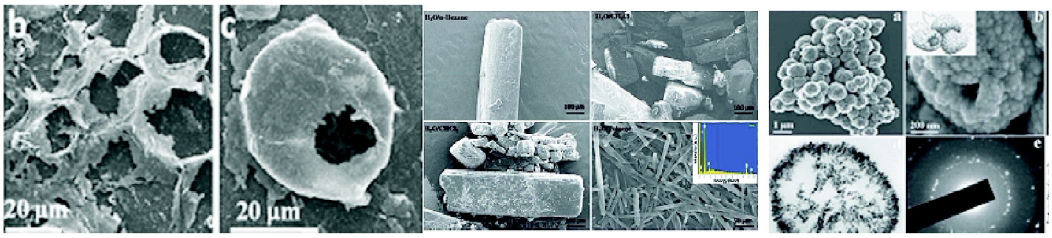


Fig. 1. SEM images of capsule, Nanorods and raspberries.

References

1. S. U. Pickering, CXCVI–Emulsions, *J. Chem. Soc. Trans.*, 1907, **91**, 2001-2021.
2. P. Pieranski, *Phys. Rev. Lett.,* 1980, **45**, 569.
3. M. Ali, S. Bora and S. K. Ghosh, *Langmuir,* 2014, **30**, 10449.
4. M. Ali, S. K. Pal, H. Rahaman and S. K. Ghosh, *Soft. Matter,* 2014, **10**, 2767.
5. M. Ali and S. K. Ghosh, *Mater. Res. Exp.*, 2015, **2**, 075010.
6. S. K. Ghosh and T. Pal, *Chem. Rev.*, 2007, **107**, 4797.
7. Y. Lin, H. Skaf, Alexander Böker, A. D. Dinsmore, T. Emrick and T. P. Russell, *J. Am. Chem. Soc.,* 2003, **125**, 12690.

Contributory Paper-10

Electrospinning and electrospraying in drug delivery and healthcare applications

Shivendu Ranjan[a] and Nandita Dasgupta[b]
[a]School of Nano Science and Technology,
Indian Institute of Technology Kharagpur,
Kharagpur-721 302, West Bengal, India
[b]International Research Center in Critical Raw Materials for
Advanced Industrial Technologies (ICCRAM),
University of Burgos, 09001 Burgos, Spain
E-mail: shivenduranjan@gmail.com

A growing interest in the use of electrospun fibres in the food industries has seen the electrospinning of biopolymers and the encapsulation of food ingredients, enzymes and other active compounds related to the food industry. Other proposed specific applications of such composites are active packaging or preservation of nutrient activity for consumption. Another benefit of electrospinning food material is the introduction of different textures and bites to the food.

The versatility of electrospinning for the fabrication of fibers out of different materials is well known. Prior to investigating electrospun fibers for use in the food industry, natural polymers such as collagen, chitosan, alginate and gelatin has already been electrospun and tested for medical applications. Later, potential food material such as zein, soy protein and whey protein, has been electrospun. However, due to difficulty in producing fibers out of these biopolymers only, other electrospinnable polymers are often added to the biopolymers prior to electrospinning. To eliminate the use of potentially harmful solvents, most companion polymers used are water soluble such as polyethylene oxide and polyvinyl alcohol.

The demonstration of electrospinning to use emulsion as the feed solution has widen the materials and encapsulation possibilities for transformation into fibers. Earlier researchers have used coconut oil as solvent for recovery of multifunctional extracts from microalga Haematococcus pluvialis (HP) and the diatom Phaeodactylum tricornutum (PT). The coconut oil enriched with β-carotene and polyunsaturated fatty acids extracts was emulsified with an aqueous solution of ulvan and pullulan blend.

Contributory Paper-11

Green technology and sustainability

Taanisha Mukhopadhyay
Department of Chemical Engineering,
Haldia Institute of Technology,
East Midnapore, Haldia
E-mail: taanisha.mukhopadhyay.862@gmail.com

Sustainable technology or green technology deals with the short-term and long-term impact of things on the environment. Green technology takes the form of recycling, renewable resources, health and safety issues, energy efficiency, and more. Green technology gives people hope to turn around pollution and the effects of climate change. It is easier to captivate clean energy from resources such as sun and water through these technologies and revolutionize the energy sector.

There are various goals and objectives of the Green Technology I'm the environment.

- It minimizes the deterioration of the environment.
- It lowers greenhouse gases (GHG) emission to zero as well as its utilization is safe and finally it enhances healthy and improved environment for all forms of life.
- It enhances the utilization of renewables.
- It saves the use of natural resources and energy.

Many green technologies aim to reduce emissions of carbon dioxide and other greenhouse gases in order to prevent climate change. Solar power is one of the most successful green technologies and is now cheaper to deploy than fossil fuels in many countries thereby affecting the environmental sustainability of the Natural Resources.

Green technology contribute to promoting sustainable development by additional parks and green spaces are created, waste management is improved, air quality is improved thanks to the replacement of classic energy based on the combustion of fossil fuels with environmentally friendly energy based on the development of renewable energy sources, etc.

The sustainable technology prevents deterioration, contamination, and other negative environmental impacts through its use or production. The technology is efficient in terms of its use of energy and resources.

Green technology is the development and application of products, equipment and systems used to conserve the environment which minimizes the negative impact from human activities[1,2]. The technology can be in the form of green buildings or renewable energy such as hydro, solar and biogas.

Green technology is important nowadays because with green tech, people can continue to harness energy from nature through solar panels, wind turbines, dams, and geothermal wells, among many others. By using alternative energy, fossil fuels will not be depleted, greenhouse gases will lessen, and global warming will slow down.

Clean technologies stand to provide significant relief to shortages in energy, water, and other natural resources, while providing a path for both developed and developing countries to address such pressing concerns as greenhouse gas emissions, deforestation, resource scarcity, and air and water pollution.The focus of green growth strategies is ensuring that natural assets can deliver their full economic potential on a sustainable basis. That potential includes the provision of critical life support services – clean air and water, and the resilient biodiversity needed to support food production and human health. Green technology helps reduce emissions, conserves water, reduces waste and consumes less energy than conventional technology. Green buildings also use materials more efficiently. The idea of green technology will help individuals conserve the earth’s renewable and nonrenewable resources. Along with this, its aim is to reduce negative impacts on the environment caused by human activity, such as pollution and global warming.

Thus New and emerging technologies could facilitate new pathways towards sustainable development that also take into consideration its economic, social and environmental dimensions.

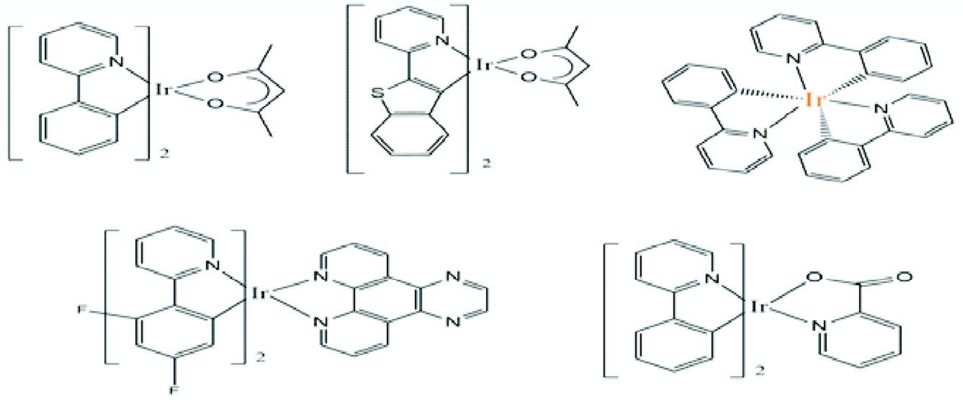
Contributory Paper-12

Bioactive cyclometallated iridium complexes containing ppy type ligands

K. C. Pradhan and S. N. Pal*
Department of Chemistry,
Utkal University,
Bhubaneswar, Odisha, India
*E-mail: kahnucharan1@gmail.com

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

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



Some cyclometalated luminescence Iridium complexes

References

1. C. Adachi, M. A. Baldo, S. R. Forrest and M. E. Thompson, *Appl. Phys. Lett.,* 2000, **77**, 6904.
2. K. H. Lee, H. J. Kang, S. O. Kim, S. J. Lee, J. H. Seo, Y. K. Kim and S. S. Yoon, *Mol. Cryst. Liq. Cryst.*, 2010, **530**, 186-195.

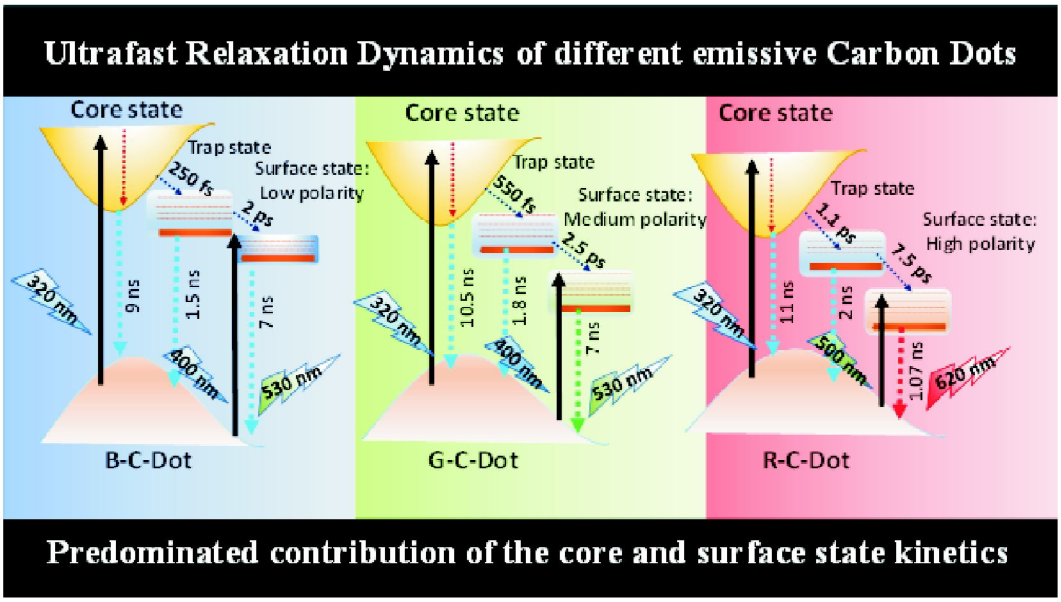
Contributory Paper-13

Exploring the origin of fluorescence of full-color light-emitting carbon dots and their carrier dynamics

Soumyadip Bhunia[a,c], Pradipta Purkayastha[a] and Somen Mondal[b]
[a]Indian Institute of Science Education and Research Kolkata,
Mohanpur-741 246, West Bengal, India.
[b]Institute of Chemical Technology, Mumbai,
Marathwada Campus, Jalna,
Maharashtra-431 203, India
[c]Indian Institute of Technology Gandhinagar,
Gandhinagar, Gujarat-382 355, India
E-mail: bitu.chem93@gmail.com

Carbon dots were gaining significant momentum in versatile fields in Physical Chemistry, Materials Chemistry, and Nanotechnology science of its birth in the carbon family, with an exponentially growing number of publications and citations. The most versatile precursors for the synthesis of C-dots were citric acid as carbon and urea as nitrogen precursors. Although there were numerous papers on these C-dots, the origin or fluorescence of blue, green, and red emissive C-dots was not still fully understood. Another important query is does green and red emissive C-dots means they will only show emission in the green and red region? Is it really possible to separate the blue emission from green and red emissive C-dots?

To resolve this existing problem, we synthesized three different C-Dots (blue, green, and red-emitting C-Dots) from the same starting materials *via* the hydrothermal method and separated them using silica column chromatography. In order to understand these mysteries, the perennial problems were tried to be solved by using steady-state, time-resolved PL, and ultrafast TA spectroscopy using highly purified C-Dots. We studied the excited-state dynamics of the differently emitting C-Dots (B-C-Dots, G-C-Dots, and R-C-Dots) in the femtoseconds-nanoseconds (fs-ns) time scale through selective excitation of the core and the surface states to reveal the different carrier relaxation processes. In this quest, we have tried to establish a concrete conclusion regarding the origin of Fluorescence in C-dots “thinking out of the box” and speaking the different languages at the cross-border of Materials Science, physical chemistry, and Photonics. Finally, the charge separation dynamics of blue-emitting carbon dots were explored in a protein biopolymer environment using hemin molecule as well as using suitable water pollutants.



References

1. S. Bhunia, N. Ghorai, S. Burai, P. Purkayastha, H. N. Ghosh and S. Mondal. *Journal of Physical Chemistry C*, 2021, **125**, 27252-27259.
2. S. Mondal, N. Ghorai, S. Bhunia, H. N. Ghosh and N. Amdursky, *Chemical Science*, 2021, **12**, 8731-8739.
3. K. Hola, M. Sudolska, S. Kalytchuk, D. Nachtigallova, A. L. Rogach, M. Otyepka, *ACS Nano*, 2017, **11**, 12402-12410.

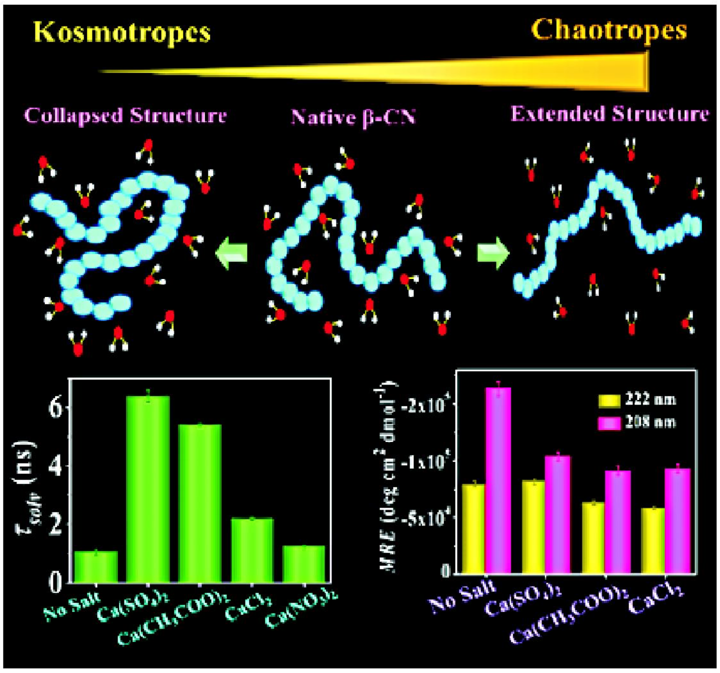
Contributory Paper-14

Role of water hydration on the formation of collapsed globule to fuzzy complex of bovine beta-casein: Effect of hofmeister series

Ushasi Pramanik and Saptarshi Mukherjee*
Department of Chemistry
Indian Institute of Science Education and Research,
Bhopal-462 066
E-mail: ushasi17@iiserb.ac.in,
*saptarshi@iiserb.ac.in

The recent burgeoning interest in Intrinsically Disordered Proteins (IDPs) aims at the disorder to order transitions due to their chameleon characteristics[1]. The dynamics and the associated solvation properties exerted by the water molecules play profound roles in the structural transitions of IDPs[2]. Salts can also modulate the stability and functional properties of proteins based on the classification by Hofmeister Series (HS)[3]. Thus, the salt-induced conformational transition of IDP and the role of water molecules during this structural switch shed interesting impacts in the biophysical research though not explored much[4,5].

Herein, we report the alterations in the conformation of beta-casein (β-CN) from its native state to a collapsed conformer and a fuzzy complex as a function of HS, based on its binding



ability with Ca^{2+} ions. A series of spectroscopic studies reveal that kosmotropic ions help the native structure of the protein to adopt a more stable state. In contrast, the chaotropes are responsible for the extended conformer[6]. Thus, the water molecules change their orientations with the structural transition of the protein in different ions. The solvation time of the protein in the presence of kosmotropes was found significantly slower (in ns time scale) compared to its native state and in the presence of chaotropes[6]. Our results dictate that the hydration shell within the collapsed state of the protein becomes more ordered and elicits slower water relaxation than the biological water and bulk water.

References and Notes

1. V. N. Uversky, Intrinsically disordered proteins and their "Mysterious" (Meta) physics, *Front. Phys.*, 2019, **7**, 10.
2. S. Arya, A. K. Singh, T. Khan, M. Bhattacharya, A. Datta and S. Mukhopadhyay, Water rearrangements upon disorder-to-order amyloid transition, *J. Phys. Chem. Lett.*, 2016, **7**, 4105.
3. S. S. Ribeiro, T. Castro, C. M. Gomes and J. C. Marcos, Hofmeister effects on protein stability are dependent on the nature of the unfolded state, *Phys. Chem. Chem. Phys.*, 2021, **23**, 25210.
4. P. Dogra, S. S. Roy, A. Joshi and S. Mukhopadhyay, Hofmeister ions modulate the autocatalytic amyloidogenesis of an intrinsically disordered functional amyloid domain via unusual biphasic kinetics, *J. Mol. Biol.*, 2020, **432**, 6173.
5. S. Wohl, M. Jakubowski and W. Zheng, Salt-dependent conformational changes of intrinsically disordered proteins, *J. Phys. Chem. Lett.*, 2021, **12**, 6684.
6. U. Pramanik and S. Mukherjee, Role of water hydration on the formation of collapsed globule to fuzzy complex of bovine beta-casein: Effect of hofmeister series. (Manuscript under preparation).

Contributory Paper-15

Coiled-coil helical nano-assemblies: Shape persistent, thixotropic and tunable chiroptical properties

Angshuman Ghosh
Kazi Nazrul University,
Asansol, Bardhaman
E-mail: ghoshangshu@gmail.com

Here, we studied the self-assembly and chiroptical properties of four C2-symmetric molecules bearing terephthaloyl (TLF C4 and TLF C12) and benzene-1,4-dicarbonyl core (BLF C4 and BLF C12). β-turn in the aggregates of TLF C4 and TLF C12 was found irrespective of the amount of water as anti-solvent in methanol (MeOH). Interestingly, chiroptical properties can be switched from β-turn to twisted β-sheet secondary structure in BLF C4 and BLF C12 beyond a certain amount of water in MeOH. Detailed studies suggested lamellar arrangement of the TLF C4 gelators with a β-turn led to the formation of right-handed coiled-coil helical fibers. However, left-handed coiled-coil twisted fibers were formed by lamellar packing (twisted β-sheet) of BLF C4. In addition, TLF C12 gel in methyl cyclohexane (MCH) revealed shape persistent gelation. Rapid dynamic equilibrium between association and dissociation of non-covalent interactions in BLF C12 gel in MCH resulted in thixotropic and, in turn, injectable behavior.

Contributory Paper-16

Imidazo[4,5-f][1,10]phenanthrolin-2-yl)phenol based Ruthenium(II) and Iridium(III) complexes analogues as hypoxia active, GSH-resistant, cytoselective and mitochondria targeting Cancer stem cell therapeutic agent

Binoy Kar and Priyankar Paira*
Department of Chemistry,
School of Advanced Sciences,
Vellore Institute of Technology,
Vellore-632 014, Tamil Nadu, India
E-mail: 2016binoychem@gmail.com
priyankar.paira@vit.ac.in

To avoid several side effects of platinum based popular anticancer drugs, tireless attempt of researchers afforded them to contemplate the way of designing the appropriate GSH resistant Ru(II)-arene complexes. Herein, we have synthesized a series of Ruthenium(II)-*p*-cymene and Iridium(III)-*Cp**-imidazo[4,5-f][1,10]phenanthrolin-2-yl)phenol complexes which act as hypoxia active and Glutathione-resistant anticancer metallotherapeutics. Complex $[Ir^{III}(Cp^*)(L5)(Cl)](PF_6)$ (**IrL5**) exhibited best cytoselectivity, GSH resistance and hypoxia effectivity in HeLa and Caco-2 cells among all the synthesized complexes. **IrL5** also exhibited high cytotoxic effect on HCT-116 CSC cell line. This complex was localized in mitochondria

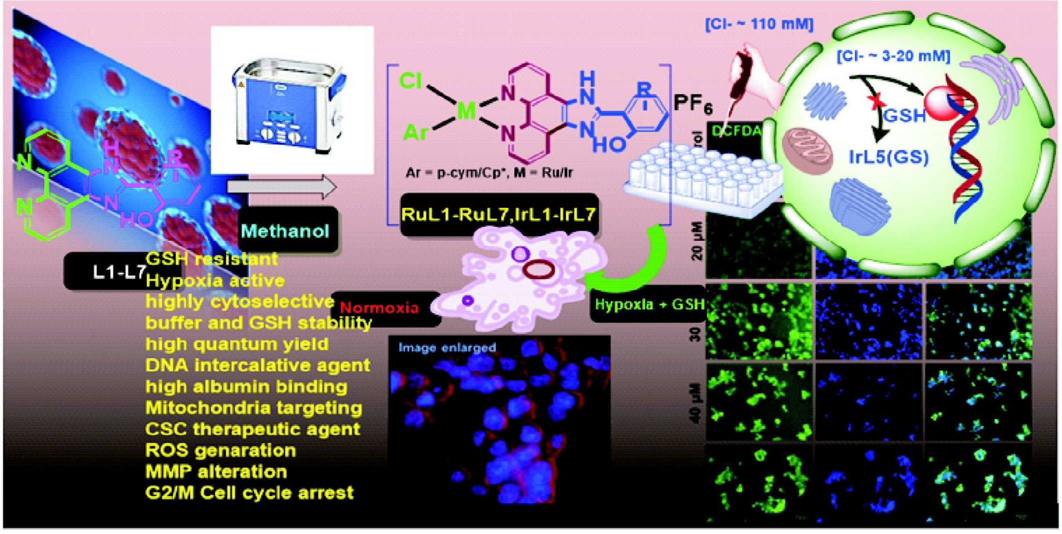


Fig. 1. Graphical representation.

and subsequent mitochondrial dysfunction was observed via MMP alteration and ROS generation on the colorectal cancer stem cells. The cell cycle analysis also established the potential of the complex to mediate a G2/M phase cell-cycle arrest.

References

1. V. Novohradsky, A. Zamora, A. Gandioso, V. Brabec, J. Ruiz and V. Marcha, Somatostatin receptor-targeted organometallic iridium(III) complexes as novel theranostic agents. *Chem. Com.,* 2017, **53**, 5523-5526.
2. Md. Hanif and C. G. Hartinger, Anticancer metallodrugs: where is the next cisplatin?. *Future Med. Chem.*, 2018, **10**, 615-617.
3. K. Suntharalingam, W. Lin, T. C. Johnstone, P. M. Bruno, Y. R. Zheng, M. T. Hemann and S. J. Lippard, A breast cancer stem cell-selective, mammospheres-potent osmium(VI) nitrido complex. *J. Am. Chem. Soc.*, 2014, **136**, 14413-14416.

Contributory Paper-17

Emulsion liquid membrane in the selective extraction of Dy

Rajib Karmakar, Pritam Singh and Kamalika Sen*
Department of Chemistry,
University of Calcutta,
92, Acharaya Prafulla Chandra Road,
Kolkata-700 009, India
E-mail: kamalchem.roy@gmail.com

This work describes the role of emulsion liquid membranes for the selective extraction of Dy(III) ion with the help of aniline yellow dye at pH 3 medium. The emulsion was prepared using different oils viz, mustard oil, coconut oil and palm oil as the organic phase. The complexation of the lanthanoides (La(III), Ce(III), Ce(IV), Pr(III), Gd(III), Sm(III) and Dy(III)) with aniline yellow (AY) and benzene azo naphthylamine (BAN) dye was studied using UV-Vis spectrophotometer at three different pH (pH 1, pH 3 and pH 5) conditions. The complexation was observed at pH 3 and 5 for only Pr(III) and Dy(III) with both the dyes having high association constant values (~10^6 M^{-1}). The emulsions were prepared using two approaches depending on the addition of the complexing agent which could be either directly in the feed solution or during emulsion formation. The emulsion liquid membrane (ELM) prepared with mustard oil showed lowest zeta potential value (–29.6 mV) compared to the coconut oil (–35.0 mV) and palm oil (–35.9 mV). Selective extraction of the Dy-AY complex was obtained for the ELM prepared with mustard oil at pH 3 medium (90 %). After extraction of the Dy-AY complex, the zeta potential decreased to –41.8 mV for the ELM. The effect of stirring time, pH of the medium and the concentration of the feeding solution have a positive correlation towards the extraction process. After the extraction process, the oil reach phase was demulsified using a mixture of organic solvents and the extracted metal ion was back-extracted with the help of cation exchange resin. 88 % of the extracted Dy could be back extracted upon demulsification.

Contributory Paper-18

A new research pathway and designed complex coordination compound for cancer arresting through cell apoptosis

A divergence towards arresting cancer cells through Ruthenium(II) binded cyclam complex with diclofenac as effective substituent and NSAIDs

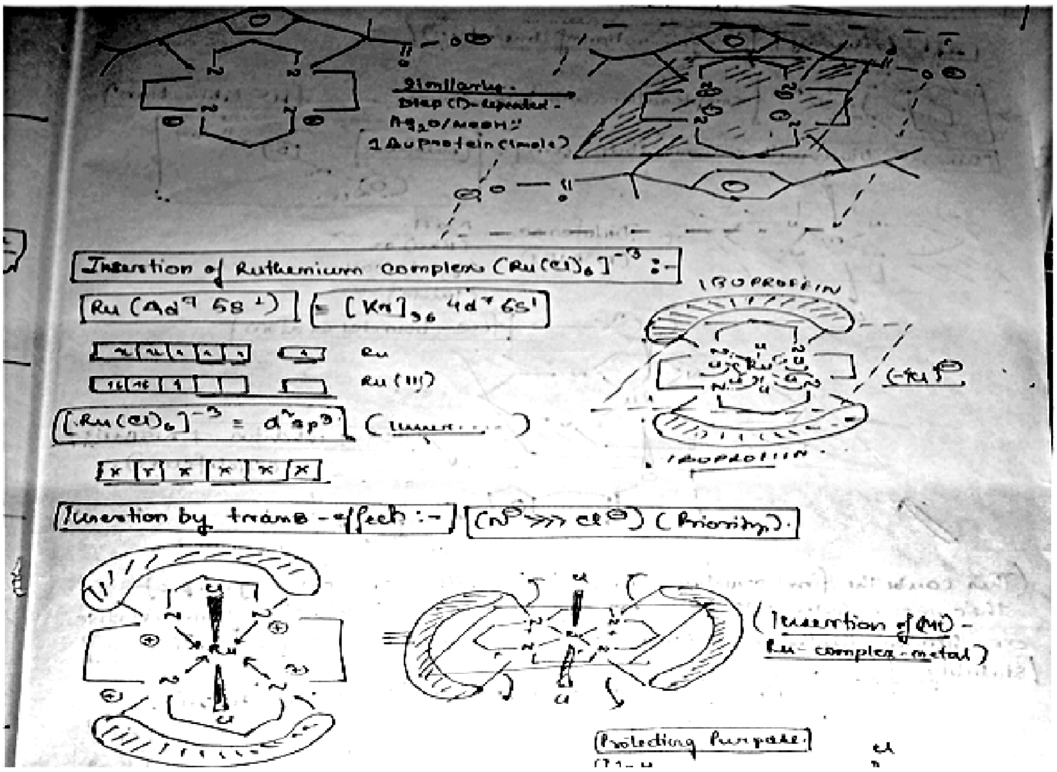
Supratik Ghosh
Department of Chemistry,
Ramakrishna Mission Vidyamandira,
Belur Math, Howrah-711 202, India
E-mail: supratikghosh1809@gmail.com

In modern 21st century the researchers and scientists have come up with a great number of ideas and technologies to combat the cancer and its disastrous effects which was not possible in olden days where fighting cancer cells and curing it was like a dream. Similarly in today's World a large no of metal complexes are used like of cobalt, Ruthenium, Nickel, platinum Binded with supramolecular chemistry elements of cyclam, Cryptands, and other Macrocyclic ligands to target the cancer cells through various processes like Dna replication blockage, Glutathione apoptosis, Fluorescence signalling etc.

The cancer treatment can be via cell apoptosis i.e. the cell death, the cancer cells can be subjected to annihilation via MoM mitochondrial potential breakdown, ROS generation, fluorescence signaling or Glutathione apoptosis. Several other factors lead to the growth of new era of anti cancer chemistry via supramolecular pathway. Here I have come up with some new ideas of designing a complex coordination compound for cancer annihilation. This compound is Based on the cyclam chemistry and it subjects Ruthenium as its base metal in (II) oxidation state. The four Coordination number out of 6 are Filled with cyclam nitrogen ends and the remaining are subjected to Arene conjugation and Diclofenac substitution as NSAIDs. An effective supposed and presumed organic mechanism is provided by me to synthesis this Coordination Compound Diclofenac which acts as Anti-inflammatory drug and resists the cancer metastatic property through processes and extensive conjugation of arene with complex increases efficiency of functioning of the complex.

The most importantly is the process which the compound adopts to act on the cancer cells. The presumed processes is that the compound follow ROS regeneration process and intrinsic Pathway of Apoptosis which is signalled through REACTIVE Oxygen Species generation and fluorescence signalling and the graphical analysis as view from journals proved that the cell activity remained constant with time. Many journals are reviewed from all around the world where the cell functioning and the Signalling process has been countered along with the apoptosis Pathway. THE PRIME Pathway is that it initiates the process though breakdown of Mitochondrial potential of membrane (MOM potential and then cytochrome diffusion to caspade activation and finally DNA replication blockage and cell death. This apoptosis is signalled though Spectroscopic analysis also to a great extend and the *Ruthenium cylam complex with diclofenac – arene system c*an be effective.

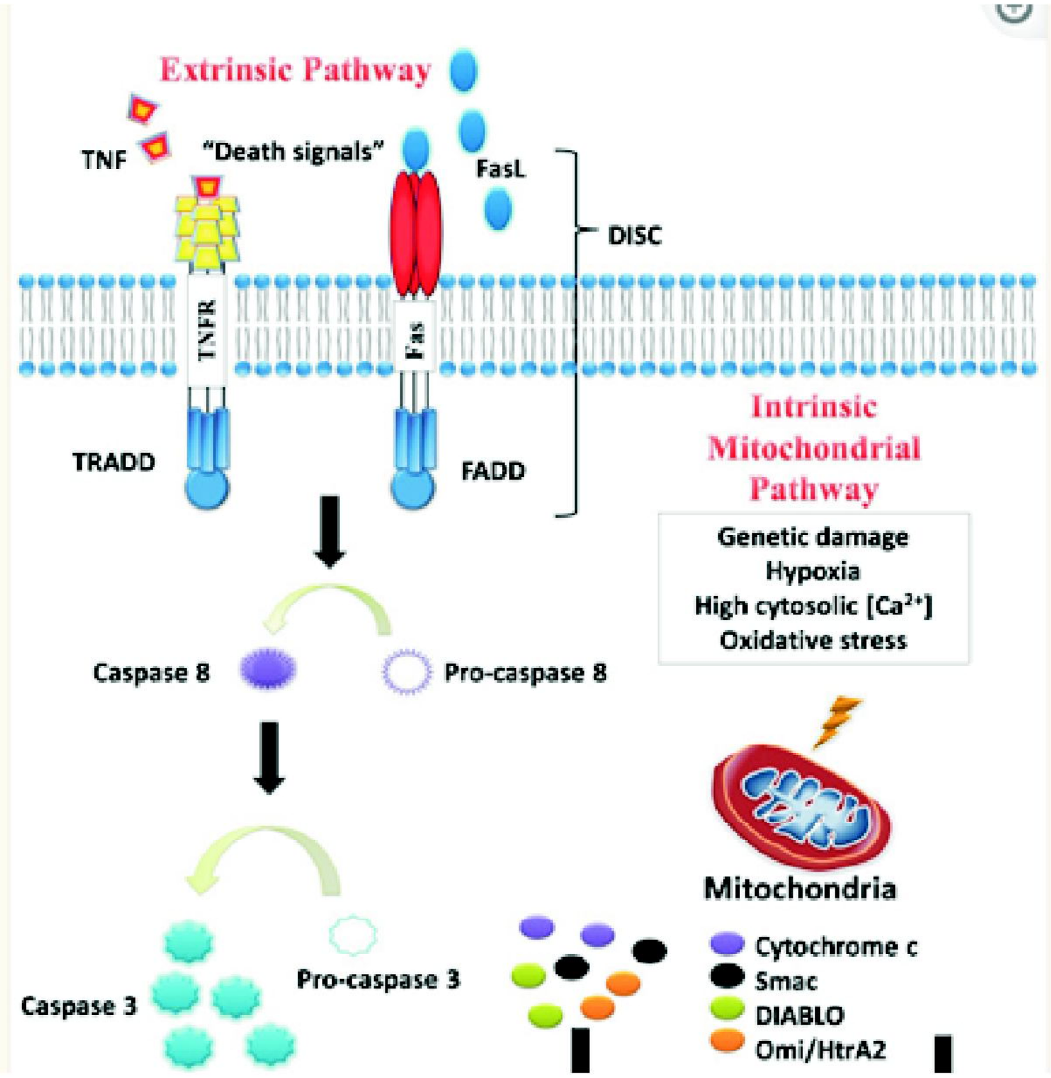
This new methodology of compound synthesis and its activities and functional process to fight the cancer can be reviewed, rechecked and analysed for proper detection of functioning process without any discrepancy and in near future this new complex coordination compound of Ruthenium can be proved a saviour against cancer if all these mechanisms and processes are analysed to be corrected as view from graphs and journals.



References

https://www.spine-health.com/treatment/pain-medication/understanding-cox-2-inhibitor-side-effects#:~:text=COX%2D2%20inhibitors%20are%20a,of%20the%20protective%20stomach%20lining

https://pubs.acs.org/doi/10.1021/acsomega.7b01512



https://pubchem.ncbi.nlm.nih.gov/compound/Diclofenac

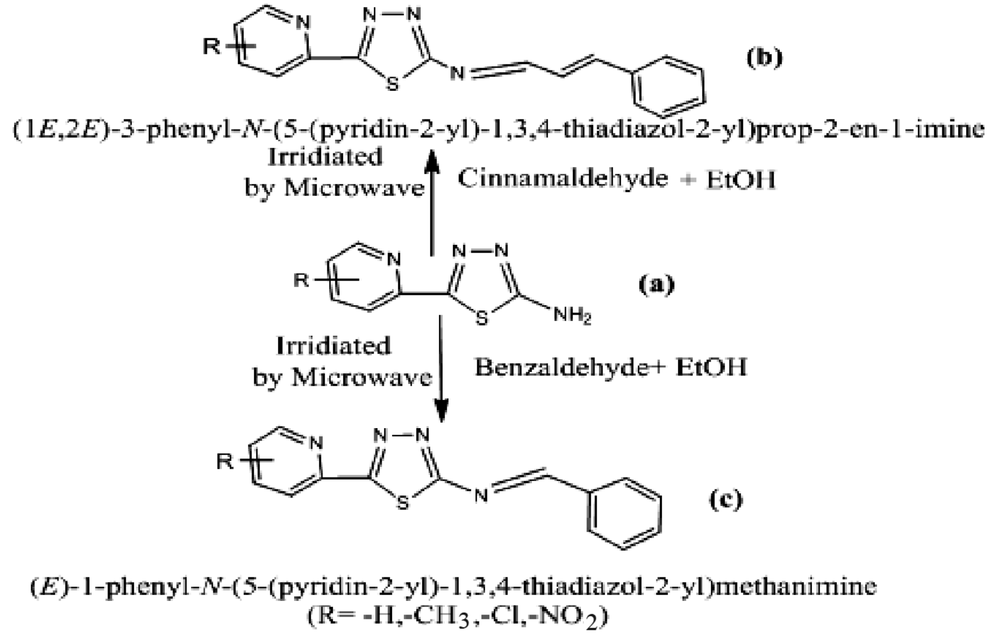
https://pubs.acs.org/doi/full/10.1021/ja3009677#

Contributory Paper-19

Green synthesis of thiadiazole based Schiff bases and their application as metallic corrosion inhibitors

Arbaj Khan, Kanha Singh Tiwari and Shailendra Yadav*
Green Chemistry Laboratory,
Department of Chemistry,
Basic Science, AKS University,
Satna-485 001, Madhya Pradesh, India
E-mail: syshailendra5@gmail.com

Schiff bases (b), (c) and their derivatives have been synthesized according to scheme A by microwave irradiation from compound (a) with maximum yield compared to conventional reflux method. The synthesized compounds were characterized by FT-IR, ^{1}H-NMR and Elemental analysis. Evaluation of corrosion inhibition efficiency of all synthesized compounds was done for mild steel in acidic media (1N HCl). It was observed that compound (b) has greater corrosion inhibition efficiency than compound (a) in case of all derivatives R= -H, -4Cl, -4NO$_2$ due to better electron donation ability of compound (b) derivatives to metal. Nitro derivative of compound b and c showed minimum inhibition efficiency while –CH$_3$ derivatives exhibited maximum inhibition efficiencies due to electron attracting power of nitro group and electron releasing power of –CH$_3$ group.



Scheme A

Contributory Paper-20

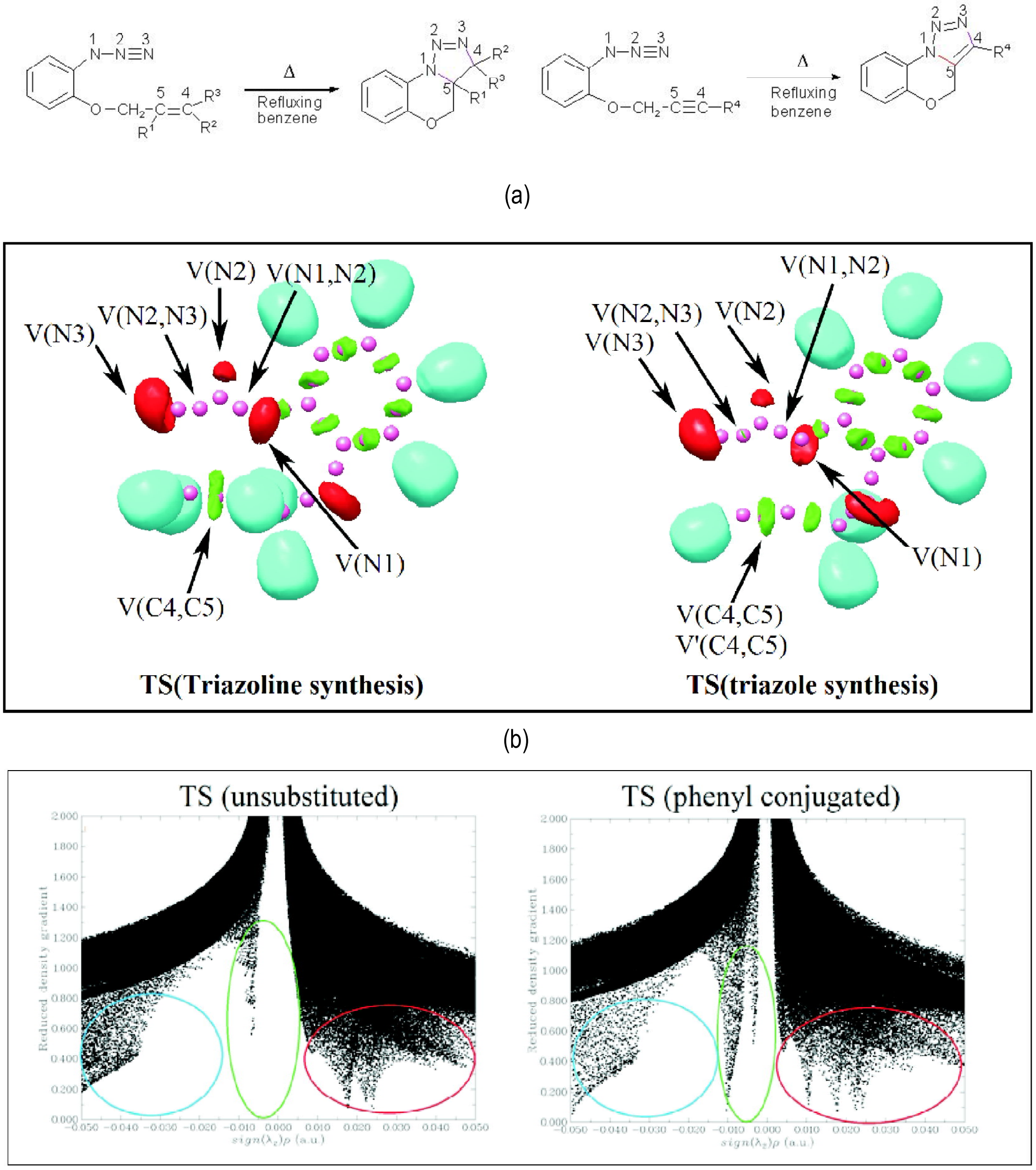
Unveiling the mechanism and substituent effects in the synthesis of fused tricyclic 1,2,3-triazolines and 1,2,3-triazoles from intramolecular [3+2] cycloadditions within the molecular electron density theory framework

Asmita Mondal and Nivedita Acharjee*
Department of Chemistry,
Durgapur Government College,
Durgapur-713 214, Paschim Bardhaman, West Bengal
E-mail: asmitamndlchem@gmail.com

Triazolines and triazoles exhibit broad range of well known pharmacological activities, consequently triggering the sincere attention of synthetic organic chemists to search for novel synthetic strategies. The intramolecular [3+2] cycloaddition (IM32CA) reactions of alkenyl and alkynyl azides serve as appealing alternatives to synthesize fused 1,2,3-triazolines and 1,2,3-triazoles, in which the reacting counterparts are suitably placed in the same molecule. Herein, the mechanism and substituent effects of these IM32CA reactions have been analysed at MPWB1K/6-311G(d,p) level using the molecular electron density theory (MEDT) proposed by Domingo in 2016[1]. MEDT[2,3] uses a set of quantum chemical tools such as electron localization function (ELF), CDFT indices, exploring potential energy surface, bonding evolution theory analysis and AIM study to analyse the reactivity, selectivity and mechanistic aspects. The present calculations revealed zwitterionic *(zw-)* type non-polar character of these IM32CA reactions following non-concerted one-step mechanism with earlier N1-C5 bond formation and Gibbs free activation energies between 27.0–31.1 kcal mol^{-1}. Interestingly, an unexpected increase in activation free energy is observed for the phenyl conjugated alkenyl and alkynyl azides relative to the unsubstituted ones, in complete agreement with the experiments. Characterization of the non-covalent interactions (NCIs) at the TSs revealed relatively denser repulsive NCI region with increase in spikes in the RDG plot for the phenyl conjugated azides.

References

1. L. R. Domingo, *Molecules,* 2016, **21**, 1319.
2. L. R. Domingo and N. Acharjee, *New J. Chem.,* 2020, **44**, 13633.
3. N. Acharjee, A. Mondal, M, Chakraborty, *New J. Chem.,* 2022, **46**, 7721-7735.



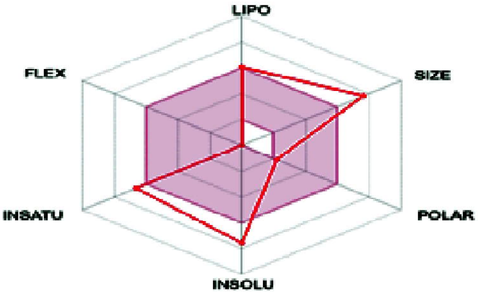
Scheme 1. (a) IM32CA reactions of alkenyl and alkynyl azides to synthesize triazolines and triazoles (b) ELF localization domains (c) RDG scatter maps at the TSs.

Contributory Paper-21

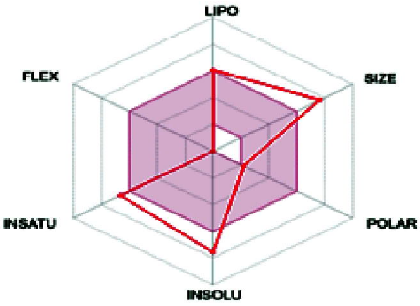
Isoelectronic and isostructural gold(III)- and platinum(II)-N-heterocyclic carbene complexes; synthesis, structure, spectral properties, electrochemistry and molecular docking studies

Lakshmikanta Maity and Joydev Dinda*
Department of Chemistry,
Utkal University, Vani Vihar,
Bhubaneswar-751 004, Odisha, India
E-mail: Joydevdinda@gmail.com
joydevdinda@utkaluniversity.ac.in

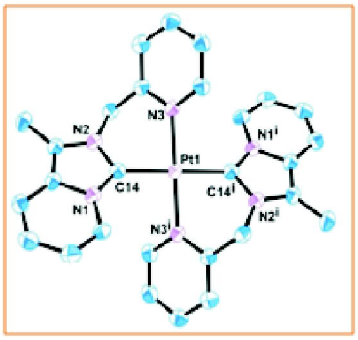
Picolyl functionalized annelated N-heterocyclic carbene proligand 1-methyl-2-(pyridylmethyl)imidazo[1,5-a]pyridin-4-ylium hexafluorophosphate, (**1**.HPF_6), and its two novel isoelectronic and isostructural complexes, viz. gold(III)-N-heterocyclic carbene complex (**2**) and platinum(II)-N-heterocyclic carbene complex (**3**) have been synthesized and characterized by several spectroscopic studies. Finally, single crystal X-ray diffraction studies revealed the



Complex-2



Complex-3



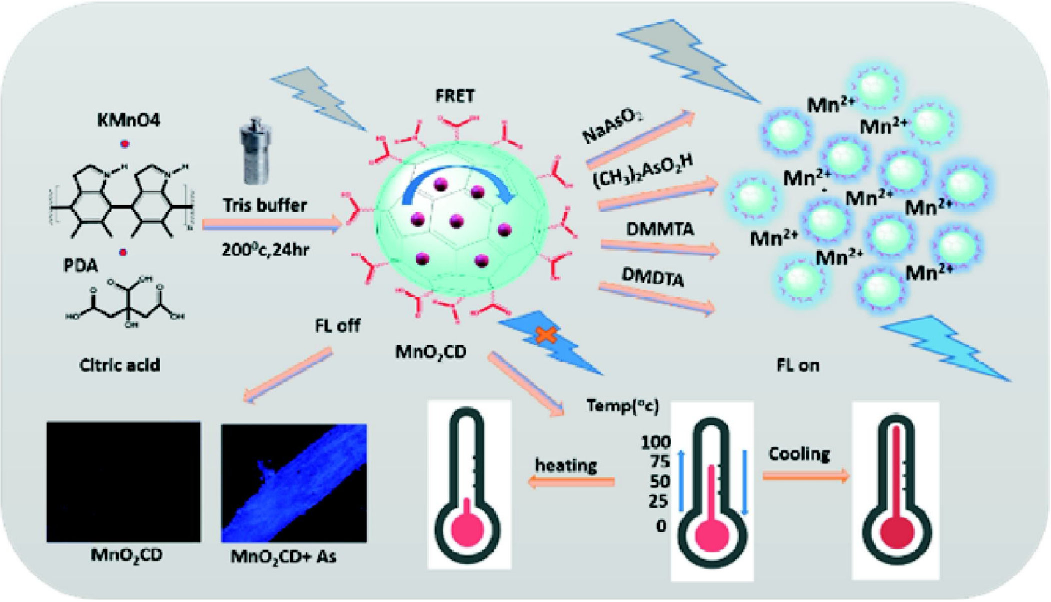
square planar geometry of both complexes **2** and **3** around respective d^8 metal ion. Both the complexes were luminescent. DFT and TDDFT studies were performed to insight into experimental findings of solid state structures and electronic properties. Cyclic voltammetric studies revealed two irreversible Au(III)→Au(I) (at -0.75 V) and Au(I)→Au(0) reductions (at –1.28 V) for Au(III)-NHC complex **2** and two electron reversible oxidation Pt(II/IV) at 0.53 V for Pt(II)-NHC complex **3**. Molecular docking analysis and pharmacokinetics studies have been performed which revealed the highest free binding energy for complex **3** with Human-DNA Topoisomerase than complex **2** and proligand **1**. HPF_6. The theoretical studies displayed the scope of the complexes to be potent drugs.

Contributory Paper-22

One-pot synthesis of MnO_2CD for multiple applications: Detection of arsenic in water, rice plant and reversible temperature sensing

Lingaraj Behera, Debasish Pati, Binod Bihari Sahu and Sasmita Mohapatra*
Department of Chemistry,
National Institute of Technology Rourkela,
Rourkela-769 008, Odisha, India
E-mail: lingarajbehera007@gmail.com

Manganese dioxide-carbon dot (MnO_2CD) composite nanoparticles of size 45 nm have been synthesized in a single step from hydrothermal decomposition of $KMnO_4$, polydopamine, and citric acid. The particles show mild emission at 425 nm at excitation wavelength 340 nm with high aqueous dispersion stability and excellent salt stability. The feeble emission property MnO_2CD arises because of fluorescence resonance energy transfer from CD to MnO_2. In presence of arsenite, the emission intensity of MnO_2CD was substantially increased because of redox reaction between MnO_2 and arsenite to give soluble Mn^{2+}. This single probe sensor shows selective and sensitive response to arsenite in the linear range of 0 to 100 nM with a detection limit of 5.75 nM. Furthermore, the probe shows satisfactory performance for turn-on detection of organoarsenic and organoarsenic compounds such as Dimethylarsenate (DMA), dimethyldithioarsinate (DMDTA), and dimethylmonothioarsinate (DMMTA). Interestingly, this sensor works well for monitoring As in a plant root vascular system through fluorescence and confocal imaging.

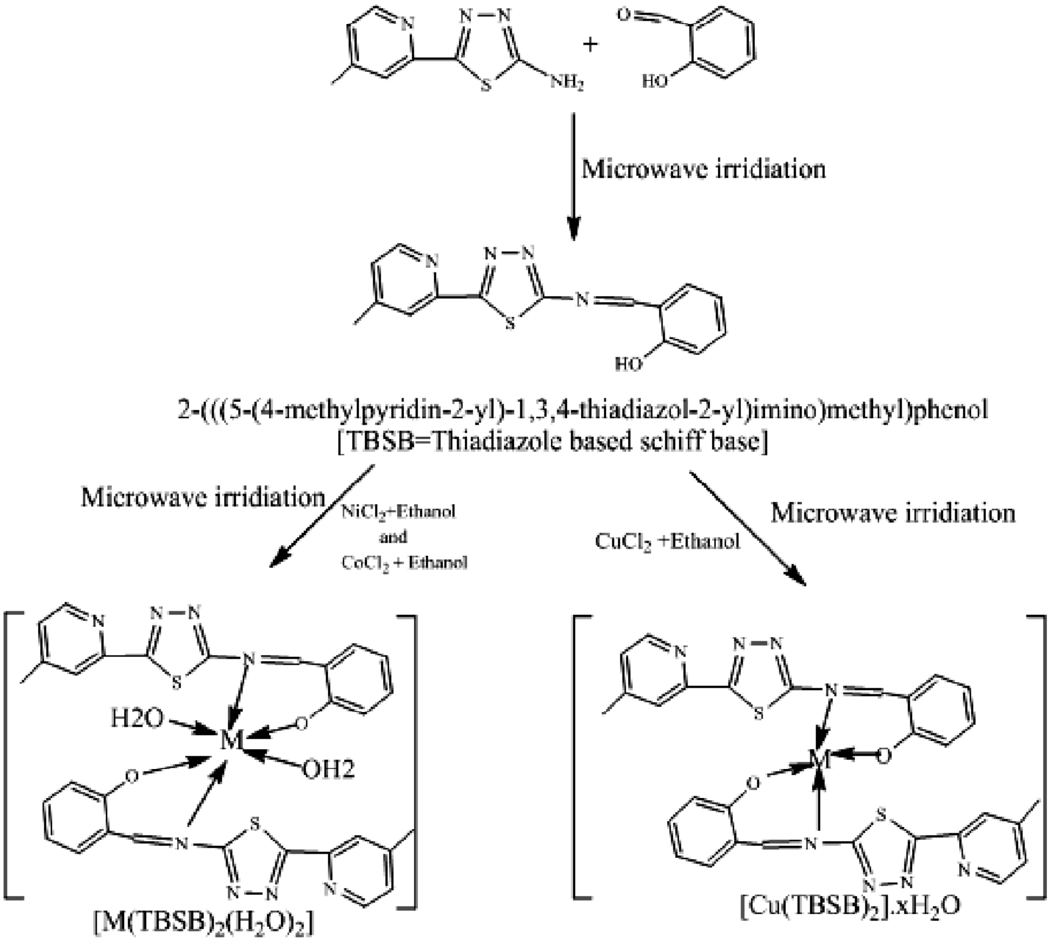


Contributory Paper-23

Synthesis and characterization of biologically active complexes of transition metals with thiadiazole based Schiff base

Sankatha Prasad Sonkar, Kanha Singh Tiwari and Shailendra Yadav*
Green Chemistry Laboratory,
Department of Chemistry,
Basic Science, AKS University,
Satna-485 001, Madhya Pradesh, India
E-mail: shailendra121282@gmail.com

In the Present synthesis work, biologically active complexes of Co(II), Ni(II), Cu(II) have been synthesized with thiadiazole based Schiff base according to scheme (a). Schiff base



was synthesized by reacting 5-(4-methylpyridin-2yl)1,3,4-thiadiazole-2-amine with salicylaldehyde by microwave assisted method . Complexes were characterized on the basis of elemental analysis, electronic spectra, FT-IR, ^{1}H-NMR, ESR and XRD analysis. Antibacterial activities of complexes, Schiff base were evaluated for *Staphylococcus aureus*, *Escherichia coli* and antifungal activities were evaluated for *Pyricularia oryzae*. It was observed that each complex exhibited greater antibacterial and antifungal activities than Schiff base against selected species.

Contributory Paper-24

CuI-Graphene nanocomposites as fluorosensors of benzaldehydes and consequent photodegradation

Debashree Das and Kamalika Sen
Department of Chemistry,
University of Calcutta,
92, Acharaya Prafulla Chandra Road,
Kolkata-700 009, India
E-mail: debashreedas2@gmail.com

Benzaldehyde and 4 methyl benzaldehyde constitute a major part of the harmful volatile organic compounds (VOCs) found in the environment. Hence, rapid and selective detection of benzaldehyde derivatives are required to minimize the environmental degradation as well as the potential hazards on human health. In this study, the surface of the graphene nanoplatelets were functionalized with CuI nanoparticles for specific and selective detection of benzaldehyde derivatives by fluorescence spectroscopy. CuI-Gr nanoparticles exhibited higher efficiency towards the detection of benzaldehyde derivatives as compared to pristine CuI nanoparticles with detection limit (LOD) as 2 ppm and 6 ppm for benzaldehyde and 4 methyl benzaldehyde respectively. The LOD values for the detection of benzaldehyde and 4 methyl benzaldehyde by pristine CuI nanoparticles were far poor and found as 89 and 18 ppm. Moreover, CuI-Gr is found to interact differentially with the benzaldehyde derivatives, which enables the sensor to distinguish between benzaldehyde and 4 methyl benzaldehyde. Fluorescence intensity of CuI-Gr nanoparticles were found to be quenched with increasing concentration of benzaldehyde while enhancement of fluorescence signal intensity of CuI-Gr was found due to the successive addition of 4 methyl benzaldehyde. This novel graphene-based sensor was also found to be highly selective for the benzaldehyde derivatives as no changes in signal were detected in presence of other VOCs like formaldehyde and acetaldehyde.

Contributory Paper-25

A small molecule inhibits GTPase activity mediated by dual protein complex of signal recognition particle (SRP) pathway

Chitra Shanbhag[a], Snehlata Saini[b], Jyotrimayee Samal[a] and Ishu Saraogi*[a,b]
Department of Chemistry[a] and Department of Biological Sciences[b],
Indian Institute of Science Education and Research, Bhopal,
Bhopal, India
E-mail: chitra16@iiserb.ac.in
ishu@iiserb.ac.in

Signal recognition particle (SRP), a ribonucleoprotein complex along with its receptor protein SR, forms a heterodimer that mediates the translocation of nascent chain polypeptides from the ribosome to the membrane translocon. This process is called co-translational protein targeting[1,2]. The essential step in this mode of protein targeting is GTPase activity mediated by the SRP-SR complex. Recent reports on SRP have put a fresh impetus on its role in several human diseases and its emerging role as an antibiotic target[3,4]. This necessitates the design and search of a small molecule inhibitor for GTPase activity driven by SRP-SR complex. In this aspect, we have checked the ability of a small molecule dynasore (a known inhibitor of dynamin GTPase) to bind to the SRP-SR complex in competition to GTP and inhibit the GTPase activity. To study this, we have utilized a colorimetric-based GTPase functional activity assay and the fluorescent nature of dynasore to assess its binding to the protein heterodimeric complex. We have shown that dynasore at an equimolar concentration to GTP, binds to protein heterodimeric complex and inhibited the GTPase activity to the basal level. Docking results of dynasore to SRP-SR complex further confirmed the binding mode of dynasore to G-domain heterodimeric interface and its interaction with necessary amino acid residues required for binding of GTP and its catalytic activity. The structure-activity relationship (SAR) based study with precursor and synthesized analogs of dynasore revealed both the precursors and the analogs of dynasore which lack catechol are inefficient in showing the inhibitory activity as similar to dynasore. Overall, our studies show the availability of the transient cavity at the G-domain interface of the SRP-SR complex, which can be targeted by small-molecules to disrupt GTPase activity[5].

References

1. I. Saraogi, D. Akopian and S. O. Shan, Regulation of cargo recognition, commitment and unloading drives cotranslational protein targeting. *J. Cell Biol.,* 2014, **205(5)**, 693-706.
2. S. O. Shan, R. M. Stroud and P. Walter, Mechanism of association and reciprocal activation of two GTPases. *PLoS Biol.*, 2004, **2(10)**.

3. S. Ghosh, S. Saini and I. Saraogi, Peptide nucleic acid mediated inhibition of the bacterial signal recognition particle. *Chem. Commun.*, 2018, **54(59)**, 8257-8260.
4. C. Bellanné-Chantelot, B. Schmaltz-Panneau, C. Marty, O. Fenneteau, I. Callebaut, S. Clauin, A. Docet, G. L. Damaj, T. Leblanc, I. Pellier, *et al.*, Mutations in the SRP54 gene cause severe Congenital Neutropenia as well as Shwachman-Diamond – like syndrome. *Blood,* 2018, **132(12)**, 1318-1331.
5. C. Shanbhag, S. Saini, J. Samal and I. Saraogi, A small molecule inhibits GTPase activity mediated by dual protein complex of signal recognition particle (SRP) pathway. (Manuscript under preparation).

Contributory Paper-26

Zn(II) based covalent organic framework: An active mesoporous catalyst for chemical incorporation of CO$_2$ under ambient conditions

Priyanka Sarkar and Sk. Manirul Islam*
University of Kalyani,
Department of Chemistry,
Kalyani, Nadia-741 235, West Bengal, India
E-mail: manir65@rediffmail.com

Removal of primary greenhouse gas carbon dioxide (CO$_2$) to valuable fine chemicals is very important for environmental remediation as the continuous accumulation of CO$_2$ in the atmosphere causes global environmental problem in all over the world[1]. We demonstrate the selective N-methylation and carbamate formation reactions *via* chemical incorporation of CO$_2$ using Zn loaded TFP-DAQ COF (Covalent Organic Framework), a mesoporous active catalyst under mild reaction condition. Selectivity of N-methylation and N-formylation reactions are readily controlled by simply varying the type of solvent.

The Zn(II)@TFP-DAQ COF catalyst is characterized by different characterization techniques like PXRD, FTIR, UV-vis spectroscopy, N$_2$ adsorption–desorption studies, FESEM and TEM images. The catalyst material exhibit pores in mesoporous region with excellent high surface area 1117.375 m²/g.

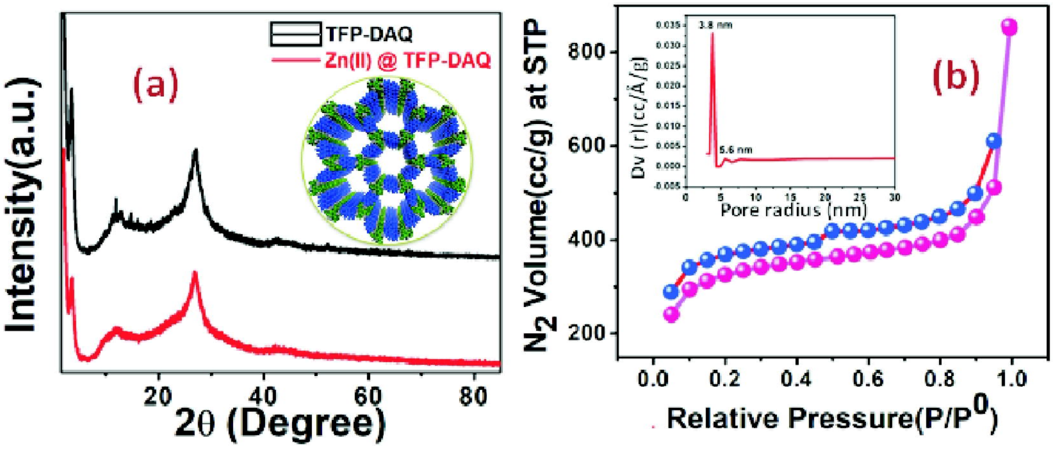


Fig. 1. (a) Powder XRD patterns of the TFP- DAQ COF and Zn (II) @ TFP- DAQ COF samples and (b) N$_2$ adsorption–desorption isotherm of Zn (II) @ TFP- DAQ COF at 77 K ; Pore size distribution plot (inset).

The synthesized material is applied as a cheap catalyst for N-methylation of secondary amines and in carbamate formation reactions which have significantly high turnover numbers (TONs) with high yields of the desired products upto 98.5% and 97% respectively with > 99% selectivity. The catalyst is found to be completely heterogeneous and reusable for multiple reaction cycles.

References

1. (a) P. Sarkar, A. Das, S. Ghosh and S. Manirul Islam, *ChemCatChem.*, 2022, e202200186;

   (b) P. Sarkar, A. H. Chowdhury, S. Biswas, A. Khan and S. M. Islam, *Mater. Today Chem.*, 2021, **21**, 100509;

   (c) P. Sarkar, S. Riyajuddin, A. Das, A. H. Chowdhury, K. Ghosh and S. M. Islam, *Mol. Catal.,* 2020, **484**, 110730.

Contributory Paper-27

Mesoporous covalent organic framework: An active photo-catalyst for reduction of carbon dioxide into formic acid under visible light

Surya Das and Sk. Manirul Islam*
Department of Chemistry,
University of Kalyani,
Kalyani, Nadia-741 235, West Bengal, India
E-mail: dassurya394@gmail.com
manir65@rediffmail.com

We have demonstrated the photocatalytic reduction of CO_2 into HCOOH using COF (Covalent Organic Framework) as a mesoporous active photocatalyst, in presence of sacrificial electron source and solvent under atmospheric pressure and visible-light irradiation[1–5]. Greater than 125 TON (turn over number) is achieved with 10 mg catalyst. The reaction cycle is dependent on the use of co-catalyst and sacrificial electron donor. In the absence of light, the reaction does not occur and can readily be controlled by light intensity variation. We have also demonstrated that a higher yield can be obtained with use of sunlight using the catalytic cycle. These results represent the path to an entirely new class of protocol for photocatalytic reduction of CO_2 using COF under visible light.

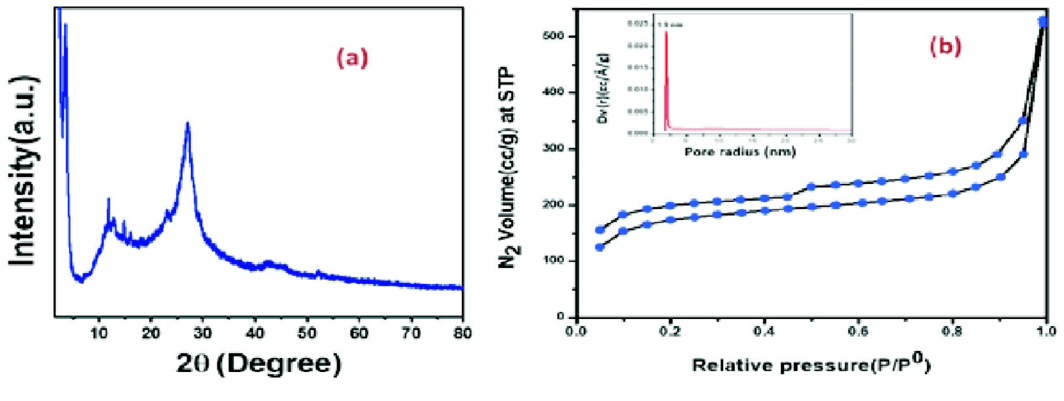


Fig. 1. (a) Powder XRD patterns of the COF and (b) N_2 adsorption–desorption isotherm of COF at 77 K; Pore size distribution plot (inset).

References

1. S. Das, I. H. Chowdhury, A. Chakraborty, M. K. Naskar, M. Sarkar and S. M. Islam, *Mater. Adv.*, 2022, **3**, 3165-3173.

2. S. Ghosh, R. A. Molla, U. Kayal, A. Bhaumik and S. M. Islam, *Dalton Trans.*, 2019, **48**, 4657-4666.
3. R. A. Molla, M. A. Iqubal, K. Ghosh and S. M. Islam, *Green Chem.*, 2016, **18**, 4649.
4. I. H. Chowdhury, A. H. Chowdhury, A. Das, A. Khan and S. M. Islam, *New J. Chem.*, 2020, **44**, 11720-11726.
5. M. Halder, Md. M. Islam, Z. Ansari, S. Ahammed, K. Sen and S. M. Islam, *ACS Sustainable Chemistry & Engineering*, 2017, **5**, 648.

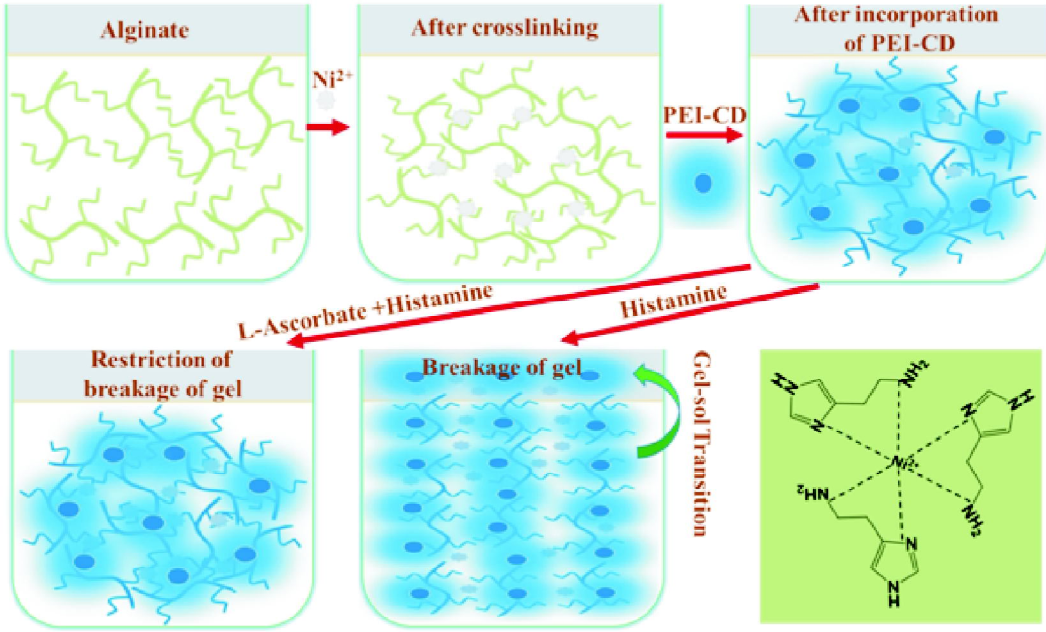
Contributory Paper-28

Selective visual detection of histamine and ascorbic acid through the rapid gel-sol transition of luminescent alginate hydrogel

Balaram Barik and Sasmita Mohapatra
Department of Chemistry,
National Institute of Technology Rourkela,
Rourkela-769 008, Odisha, India
E-mail: balarambarik2@gmail.com

A fluorescent hydrogel has been synthesized by crosslinking sodium alginate with Ni^{2+} in the presence of PEI-derived carbon dots. Such a hydrogel shows a quick selective visual response towards histamine through rapid gel-to-sol transition followed by the release of CD into the sol solution. The amount of histamine can be quantified by measuring the fluorescence intensity of sol solution at an excitation wavelength 3 360 nm. The sensor's detection limit in the turn-on intensity mode goes up to 0.63 nm. Utilizing the detoxification reaction of histamine by ascorbic acid, the present sensing platform has been explored to detect ascorbic acid. Due to low-cost and easy synthesis, such hydrogel-based fluorescent chemosensors are potentially suitable for monitoring histamine in serum and fish samples.

Graphical abstract

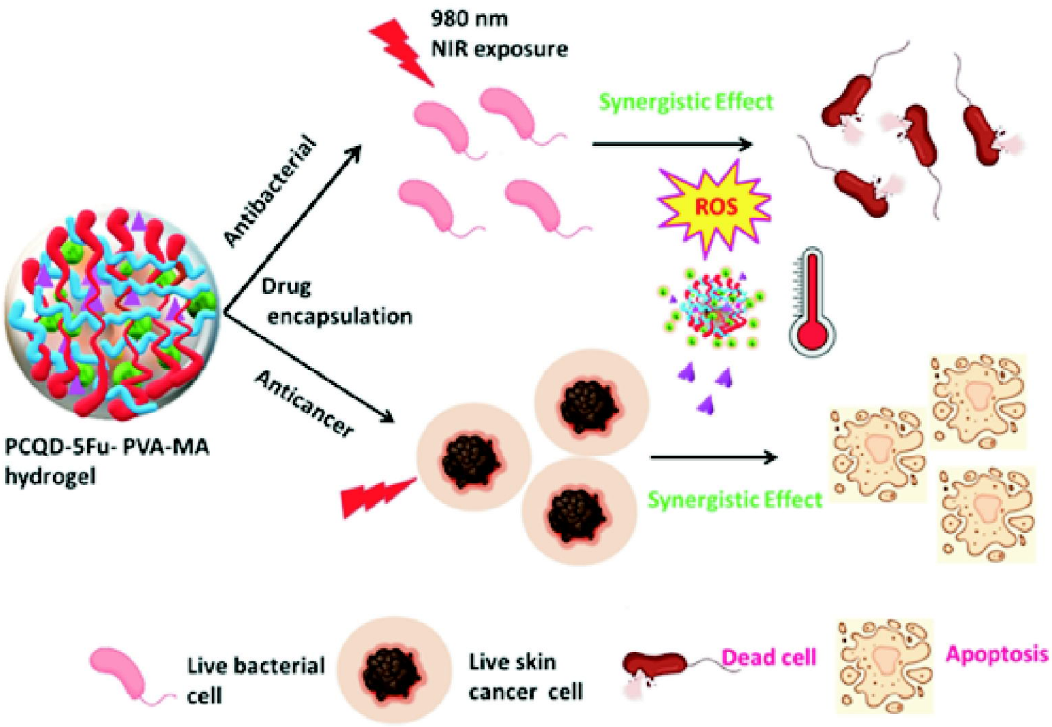


Contributory Paper-29

Papaya-derived carbon-dot-loaded fluorescent hydrogel for NIR-stimulated photochemotherapy and antibacterial activity

Snigdharani Panda, Bibek Chaw Pattnayak, Priyanka Dash,
Bismita Nayak and Sasmita Mohapatra*
Department of Chemistry,
National Institute of Technology Rourkela,
Rourkela-769 008, Odisha, India
E-mail: bibek.chawpattnayak@gmail.com

The improper use of antibiotics results in the emergence of drug-resistant microbes which is a serious concern to public health. Here, an NIR-stimulated fluorescent antibacterial gel has been formulated by encapsulating papaya leaf-derived carbon dots (PCQDs) in a thermosensitive PVA-melamine hydrogel. This antibacterial gel can release anticancer drug 5-Fu in a spatiotemporal and dosage-controlled manner under the exposure of a 980 nm NIR laser. PCQDs can precisely generate the photothermal effect and reactive oxygen species (ROS) under NIR which induce a significant antibacterial activity in both Gram-positive and



Gram-negative bacteria in a controlled manner. At the same time, a customized delivery of 5-Fu minimizes the side effect of the drug. Consequently, this innovatively designed fluorescent gel exhibited an antimicrobial effect and can act as a promising material for the NIR-responsive release of anticancer drug 5-Fu as demonstrated in B16F10 melanoma cells.

Contributory Paper-30

Photodegradation of carcinogenic organic dyes by 1D supramolecular Cu(II) complex

Ribhu Maity and Bidhan Chandra Samanta*
Department of Chemistry,
Mugberia Gangadhar Mahavidyalaya,
Bhupatinagar, Purba Medinipur
E-mail: maityribhuju@gmail.com

In the present study, the vital role of supramolecular interactions in determining the supramolecular layer architecture of heteroleptic Cu(II) complex $[Cu(L)(imid)(ClO4)]_n$ synthesized from ortho-vaniline based Schiff base and imidazole co-ligands has been investigated through a detailed study of Hirshfeld surface analysis. The synthesized Cu(II) complex efficiently degrades methylene blue (MB) (35%) and ethidium bromide (EB) (38%) dyes at 290 minutes under sunlight irradiation. The complex exhibited the highest degradation efficiency of about 95–96% after 48 hours of sunlight exposure demonstrating potentiality of this supramolecular copper(II) complex in effective photo degradation against MB and EB organic dye under sunlight with a significant appliance of it in wastewater treatment and purification.

Contributory Paper-31

Antisense PNA mediated inhibition of bacterial signal recognition particle system: A novel antibacterial strategy

Snehlata Saini[a], Sudipta Ghosh[b] and Ishu Saraogi*[a,b]
[a]Department of Biological Sciences, [b]Department of Chemistry,
Indian Institute of Science Education and Research Bhopal,
Bhauri, Bhopal Bypass Road,
Bhopal-462 066, Madhya Pradesh, India
E-mail: snehlatasaini@iiserb.ac.in

The upsurge of antibiotic resistance in pathogenic bacteria is a global health concern[1]. In pursuit of new antibacterial strategies, we have identified bacterial signal recognition particle (SRP) pathway as a potential antibacterial target[2]. It mediates the co-translational transport of nascent proteins to plasma membrane, and is essential for bacterial cell survival[3–4]. We aimed to inhibit an important RNA-protein interaction by antisense peptide nucleic acids (PNAs) to disrupt the functional SRP cycle in bacteria. *In vitro* studies confirmed that the designed PNAs specifically inhibited the RNA-protein interaction, leading to the inhibition of SRP mediated GTP hydrolysis. *In vivo* studies showed that the designed PNA effectively inhibited *E. coli* bacterial cell growth by selectively targeting 4.5S RNA. We further demonstrated the inhibition of several other bacterial strains using same strategy. This study confirms the cellular target of the designed PNA, and validates SRP as a broad spectrum antibacterial therapeutic.

Further, we studied the molecular details of the RNA-PNA interaction to understand the importance of target site selection for developing better antisense molecules[5]. One of the PNAs has a homo-pyrimidine sequence, capable of forming triplexes with homo-purine RNA. The other PNA having a mixed-base sequence can only form duplex. Biophysical assays at pH 7.0 revealed the formation of higher order structure in case of homo-pyrimidine PNA, which was further confirmed as a triplex, whereas the mixed-base PNA was found to form a duplex with RNA. *In vitro* GTPase assay showed dose-dependent inhibitory effect of the homo-pyrimidine, but not mixed-base PNAs on SRP mediated GTP hydrolysis. Thus, our results show that the formed triplex by homo-pyrimidine PNAs exhibits significant effect on RNA functionality as compared to mixed-base PNA and suggest the importance of understanding the target site selection in order to develop better antisense molecules to target bacterial SRP system.

References

1. M. F. Chellat, L. Raguz and R. Riedl, Targeting antibiotic resistance. *Angew. Chem. Int. Ed. Engl.,* 2016, **55(23)**, 6600-6626.
2. S. Ghosh, S. Saini and I. Saraogi, Peptide nucleic acid mediated inhibition of the bacterial signal recognition particle. *Chem. Commun.*, 2018, **54(59)**, 8257-8260.
3. R. J. Keenan, D. M. Freymann, R. M. Stroud and P. Walter, The signal recognition particle. *Annu. Rev. Biochem.*, 2001, **70**, 755-775.
4. S. Brown and M. J. Fournier, The 4.5S RNA gene of *Escherichia Coli* Is essential for cell growth. *J. Mol. Biol.*, 1984, **178(3)**, 533-550.
5. S. Saini, S. Ghosh and I. Saraogi, Deciphering the effect of designed homo-pyrimidine and mixed-base PNAs on bacterial 4.5S RNA structure and functionality (Manuscript under preparation).

Contributory Paper-32

Rapid detection of pathogens using biocompatible silver nanoparticles as a sensor by using FTIR spectroscopy

Amar Ghosh and Ujjal Kumar Sur*
Department of Chemistry,
Behala College,
University of Calcutta,
Kolkata-700 060, West Bengal, India
E-mail: uksur99@yahoo.co.in

Fourier transform infrared (FT-IR) spectroscopy is a physico-chemical method based on measurement of vibration of a molecule excited by IR radiation at a specific wavelength in the range of 400–4000 cm^{-1}. FT-IR spectra of bacterial cells can be used to analyze their molecular segments such as total composition with including proteins, fatty acids, carbohydrates, nucleic acids, and lipopolysacharides. In this paper, we have reported an eco-friendly green protocol for the room temperature one-step facile synthesis of biocompatible silver nanoparticles (AgNPs) by the reduction of aqueous silver ions using *Murraya koenigii* leaf extract as the abundant source of reducing and stabilizing agents. AgNPs are used to treat in the bacterial broth (pathogens such as *Staphylococcus aureus* and *Vibrio cholerae*) and then measured the FT-IR spectra in presence and absence of AgNPs. What would be the change the moieties on treatment of which different fragmentations of AgNP-pathogens, clearly confirmed that rapid detection of such pathogens in low concentration and suitable for a fast real-time monitoring, using FT-IR spectroscopy as an optical transduction method. FT-IR spectroscopy is a reliable, rapid and economic technique which could be explored as a routine diagnostic tool for bacterial analysis by the food industry, diagnostic laboratories, and public health authorities. This chapter highlights the principles of FT-IR spectroscopic analysis of bacteria, the advantages and disadvantages of FT-IR applied to bacterial analysis, spectral manipulation, statistical analysis of spectra, and applications in pathogen detection.

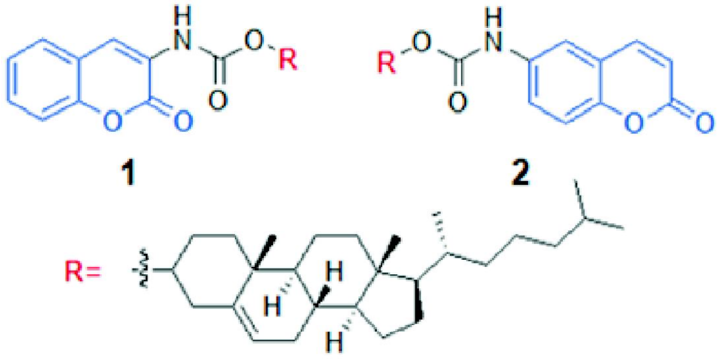
Contributory Paper-33

Positionally isomeric coumarin carbamates: Structure-gelation study, F^- recognition, dye removal and excellent oil-spill recovery

Rameez Raza, Subhasis Ghosh and Kumaresh Ghosh*
Department of Chemistry,
University of Kalyani,
Kalyani-741 235, India
E-mail: ghosh_k2003@yahoo.co.in
kumareshchem18@klyuniv.ac.in

Design and synthesis of simple Low Molecular Weight Gelators (LMWGs), capable of forming supramolecular gels, draw considerable attention because of their broad applications as soft materials in light capturing systems, drug delivery, optical sensors, catalysis and environmental remediation etc.[1]. Supramolecular gels of LMWGs arise from noncovalent force mediated self-assembly of the gelators into long fibers[1,2]. At a particular concentration, these fibers are either entangled or branched in some manner to set up a 3D-network into which solvent molecules are entrapped and immobilized to form the viscoelastic gel. In creating such 3D-network, the gelator's structure has the pertinent role. The suitable functional groups in a gelator structure influence the aggregation and represent a macroscopic manifestation. In the event, the positional alteration of the functional group that results in an isomeric structure sometimes exhibits marked effect in gelation, morphology and properties of the gel[3]. Studies on such structure–gelation relationship provide the understanding of the gelation mechanism along with other attributes in gel chemistry.

During our ongoing research in supramolecular gel[4], we wish to report here two structurally simple coumarin-based isomeric gelators **1** and **2** which show different gelation behaviors in organic solvents. The gelation condition, morphology and viscoelastic nature of the gels of **1** and **2** are varied with change in position of the functional group around the coumarin motif. While **2** formed gel in CH_3CN, under the condition compound **1** was reluctant to give gel. No gel formation was achieved in polar solvents. Both **1** and **2** was gelled in toluene with different minimum gelation concentrations (mgc). Toluene gels with dissimilar morphologies and viscoelastic properties exhibit different anion responsive characters, oil-spill recovery and dye adsorption. All these are to be focused in the poster.



1 **2**

References

1. (a) D. K. Smith, *Royal Society of Chemistry*, *Cambridge*, 2018, 300-371;

   (b) R. Xing, K. Liu, T. Jiao, N. Zhang, K. Ma, R. Zhang, Q. Zou, G. Ma and X. Yan, *Advanced Materials*, 2016, **28**, 3669;

   (c) C. Rizzo, S. Marullo, F. Billeci and F. D'Anna, *Eur. J. Org. Chem.*, 2021, 3148.
2. L. Meazza, J. A. Foster, K. Fucke, P. Metrangolo, G. Resnati and J. W. Steed, *Nat. Chem.*, 2013, **5**, 42.
3. (a) A. Dawn, J. Pajoubpong, A. Mesmer, M. Mirzamani, L. He and H. Kumari, *Langmuir*, 2022, **38**, 1705;

   (b) T. Wang, Y. Li, F. Shen, J. Ren and X. Yu, *Applied Surface Science*, 2020, **513**, 145814.
4. (a) S. Ghosh, P. Jana and K. Ghosh, *Anal. Methods*., 2021, **13**, 695;

   (b) S. Ghosh, S. Ghosh, N. Baildya and K. Ghosh, *New J. Chem.*, 2022, **46**, 8817;

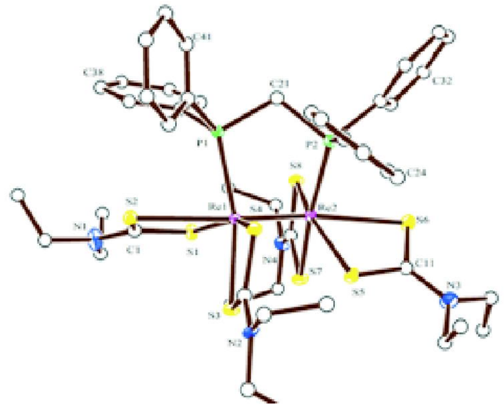
   (c) S. Ghosh Roy, A. Kumar, N. Misra and K. Ghosh, *Mater. Adv.*, 2022, https://doi.org/10.1039/D2MA00358A.

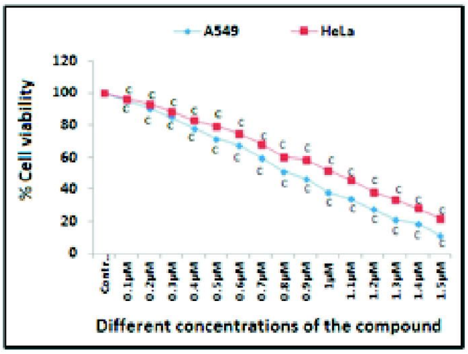
Contributory Paper-34

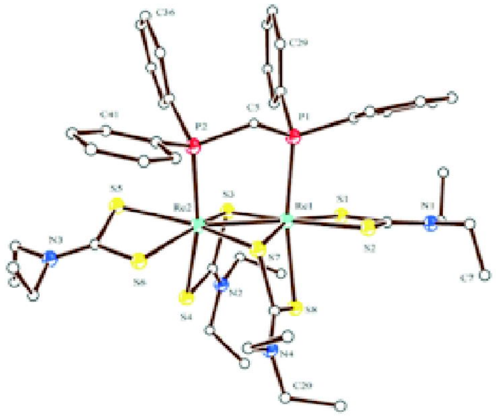
Dirhenium complexes incorporating the dithiocarbamato ligands: Spectroscopic, structural and computational studies

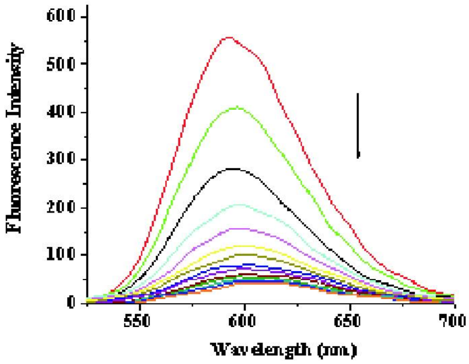
Purnananda Garu, Suman Mandal and Swarup Chattopadhyay*
Department of Chemistry,
University of Kalyani,
Kalyani-741 235, Nadia, West Bengal, India
E-mail: icskc@klyuniv.ac.in

The biological and therapeutic properties of dithiocarbamate compounds have fuelled the interest in developing the chemistry of this ligand. Only a few dithiocarbamate complexes of dirhenium have been reported. In pursuit of our general interest on the chemistry of dirhenium, we have been investigating the fundamental chemistry of dirhenium incorporating different dithiocarbamate ligands. The reason for this investigation is that the dithiocarbamate ligands have not been extensively applied to the dirhenium chemistry. In the course of this investigation we have discovered that sodium salts of dimethyldithiocarbamate (L_{Me}), diethyldithiocarbamate (L_{Et}) and pyrrolidinedithiocarbamate (L_{Pyr}) react with the double–bonded diamagnetic dirhenium(III,III) complex $Re_2(\mu\text{-dppm})_2(\mu\text{-Cl})_2Cl_4$ (dppm = $Ph_2PCH_2PPh_2$) in refluxing ethanol to afford the diamagnetic substitution products of the type $[Re_2(\mu\text{-dppm})(\eta^2\text{-}L_R)_2(\mu\text{-}\eta^2\text{-}L_R)_2](PF_6)_2$, where L_R represents the dithiocarbamato ligands. These are the first examples of dirhenium(III,III) complexes that contain bridging dithiocarbamato ligand along with the dppm ligand. In another study we have discovered that sodium salts of L_{Me}, L_{Et} and L_{Pyr} react with the triply bonded dirhenium (II,II) complex $Re_2(\mu\text{-}Ph_2PCH_2PPh_2)_2Cl_4$ to afford the products of the type $Re_2(\mu\text{-}Ph_2PCH_2PPh_2)(L_R)_4$. These are the first examples of dithiocarbamato chelated dirhenium complexes with a Re_2^{4+} core containing $Ph_2PCH_2PPh_2$ ligand. The spectral (IR, UV-vis, NMR, ESI-MS) and electrochemical properties of the complexes are reported. The identity of the complexes has been established by single-crystal X-ray structure determination. The electronic structure and the absorption spectra of the complexes are scrutinized by density functional theory (DFT) and time-dependent DFT (TD-DFT) analyses. The complexes were tested for their ability to exhibit DNA-binding activity. The antifungal and antiproliferative properties of the complexes were also studied.









References

1. S. Mandal, S. Mallick, P. Garu, J. Chowdhury, S. Banerjee, S. Sen, K. Sarkar and S. Chattopadhyay, *Polyhedron* 2021, **207**, 115373.
2. S. Mallick, P. Garu, J. Chowdhury, R. Saha and S. Chattopadhyay, *Polyhedron,* 2021, **208**, 115422.
3. S. Mandal, S. Mallick, P. Garu, J. Chowdhury, A. Samadder, J. Das, A. R. Khuda-Bukhsh and S. Chattopadhyay, *New J. Chem.*, 2020, **44**, 4081.

Contributory Paper-35

Silver based nanoparticles for biomedical applications

Shagufta Haque, Bonda Rama Rao, Caroline Celine Norbert and Chitta Ranjan Patra*
Department of Applied Biology,
CSIR-Indian Institute of Chemical Technology,
Uppal Road, Tarnaka,
Hyderabad-500 007, Telangana State, India
Academy of Scientific and Innovative Research (AcSIR),
Gaziabad-201 002, Uttar Pradesh, India
E-mail: crpatra@iict.res.in

Silver-based nanoparticles are explored for various biomedical applications due to their unique physico chemical properties. Very recently, our group has developed and designed two different types of silver based nanomaterials (AgZE: bio-synthesized silver nanoparticles and SNPNPs: silver nitroprusside nanoparticles)[1,2]. The AgZE is synthesized by reducing silver nitrate solution using *Zinnia elegans* ethanolic leaf extract[1]. On the other hand, SNPNPs are synthesized by the interaction of silver nitrate and sodium nitroprusside[2].

The AgZE shows biocompatibility observed by both *in vitro* assays and *in vivo* experiments. Cytotoxicity study are carried out by AgZE towards several cancer cell lines. The mechanism behind the anticancer activity of AgZE on human glioblastoma cell line is illustrated through various *in vitro* assays. *In vivo* anticancer activity of AgZE is exhibited through inhibition of blood vessel formation using CAM assay. Additionally, AgZE upon intraperitoneal injection in C57BL/6J mice showed fluorescence in the NIR region (uniqueness of AgZE).

Another silver-based nanomaterials (SNPNPs) impregnated on cotton fabrics (SNPCFs) that exhibits photo inertness, improved water contact angle and longer antibacterial activity after several washings[2]. The SNPCFs showed efficient wound healing activity in C57BL/6J mice. Overall, these silver nanoparticles could be used for various biomedical applications (anti-microbial, anti-cancer, NIR based imaging) in near future.

References

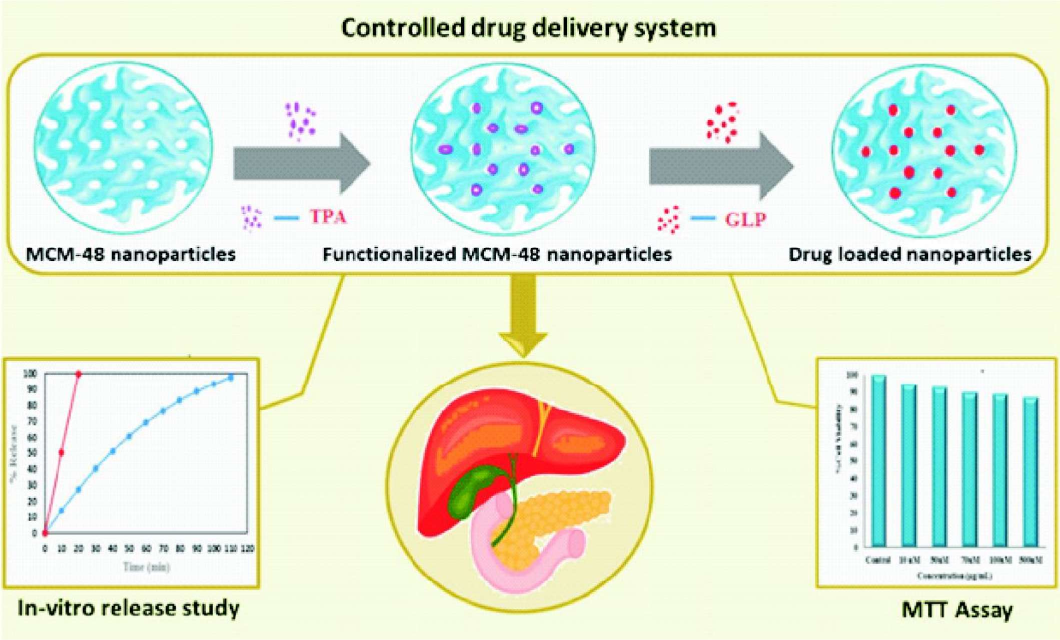
1. S. Haque, C. C. Norbert, R. Acharyya, S. Mukherjee, M. Kathirvel and C. R. Patra, *Cancers*, 2021, **13(23)**, 6114.
2. B. R. Rao, R. Kumar, S. Haque, J. M. Kumar, T. N. Rao, R. V. Kothapalli and C. R. Patra, *ACS Applied Materials & Interfaces*, 2021, **13(9)**, 10689-10704.

Contributory Paper-36

Designing of inorganic based nano drug delivery system for treatment of Diabetes Mellitus

Debatrayee Dasgupta and Anjali Patel*
Department of Chemistry,
Faculty of Science,
The Maharaja Sayajirao University of Baroda
Vadodara-390 002, India
E-mail: depuja79@gmail.com

Glipizide(GLP), a poorly soluble sulphonyl urea drug is used to treat diabetes mellitus. Because of its poor solubility and short half-life, the development of controlled delivery strategies could result in significant clinical benefits. Many such drug delivery systems (DDS) for GLP have been already studied, including microspheres, polymers, osmotic pump systems, liposomes, hydrogels, and emulsifiers. In this regard, mesoporous silica nanoparticles (MSN) has been investigated as DDS to increase the solubility as well as dissolution profile of glipizide due to unique properties like high surface area, ordered porosity and adsorption capacity. Besides that, functionalizing the MSN surface may increase drug surface interaction that will control the release mechanism. In the present work, MCM-48 nanoparticles (nMCM-48) was synthesised, functionalized and capped using 12-tungstophosphoric acid (TPA), a



Keggin type of Polyoxometalates. Different types of DDS have been prepared for e.g. first the drug was loaded in nMCM-48 and capped by TPA. All the synthesized DDS were characterized by various techniques. *In vitro* release study of GLP was carried out and compared with release profile of marketed formulation (Glynase). Results show that TPA acts better as a functionalizing agent than as a capping agent and plays an important role in the controlled release of GLP. Furthermore, the MTT Assay demonstrates that the carrier is non-toxic.

Reference

1. Y. V. Simos, K. Spyrou, M. Patila, N. Karouta, H. Stamatis, D. Gournis, E. Dounousi and D. Peschos, *Asian J. Pharm. Sci.*, 2021, **16**, 62-76.

Contributory Paper-37

Structural exploration and protein binding efficiencies of binuclear dioxidomolybdenum(VI) complexes constructed from ONO chelator and linear N-N ditopic spacer

Oiendrilla Sarkar[a], Malini Roy[a], Debanjana Biswal[a], Nikhil Ranjan Pramanik*[b], Suvendu Paul[c], Michael G. B. Drew[d] and Syamal Chakrabarti*[a]
[a]Department of Chemistry,
University College of Science,
92, AcharyaPrafulla Chandra Road,
Kolkata-700 009, West Bengal, India
[b]Department of Chemistry,
Bidhannagar College, EB-2, Sector-1, Salt Lake,
Kolkata-700 064, India
[c]Department of Chemistry,
University of Kalyani, Kalyani,
Nadia-741 235, West Bengal, India
[d]Department of Chemistry,
The University of Reading, Whiteknights,
Reading RG66AD, UK
E-mail: oiendrilla.sarkar@gmail.com

The present study describes the syntheses, spectroscopic characterizations and crystal structures of two binuclear dioxidomolybdenum(VI) complexes of general formula $[MoO_2L]_2$(N-N) with ONO donor ligands obtained by the condensation of benzoyl acetone with salicylhydrazide (H_2L^1) and anthranylhydrazide (H_2L^2) and spacer 1,2-bis(4-pyridyl)ethene (bpe). The crystal structures of these complexes have been solved by single crystal X-ray crystallography. Both the complexes (**1** and **2**) are centrosymmetric and each Mo centre exhibits a distorted octahedral geometry. The complexes give rise to 3D supramolecular architectures with the formation of cavities *via* hydrogen bonding and C-H$\cdots\pi$ stacking interactions.

Supportive DFT calculations are carried out to compare the structural parameters of the complexes with the experimental data and energy of frontier molecular orbitals are also calculated. The intermolecular interactions in the crystal structures are also studied by the Hirshfeld surface analysis. The redox behavior of complexes has been examined by cyclic voltammetry. The binding affinity and binding mode of the complexes towards BSA has been explored by absorption and fluorescence titration method. Both the complexes exhibit fluorescence resonance energy transfer from protein to the complexes. Time resolved fluorescence measurements along with the molecular docking studies are carried out to get a deeper insight into the binding mechanism.

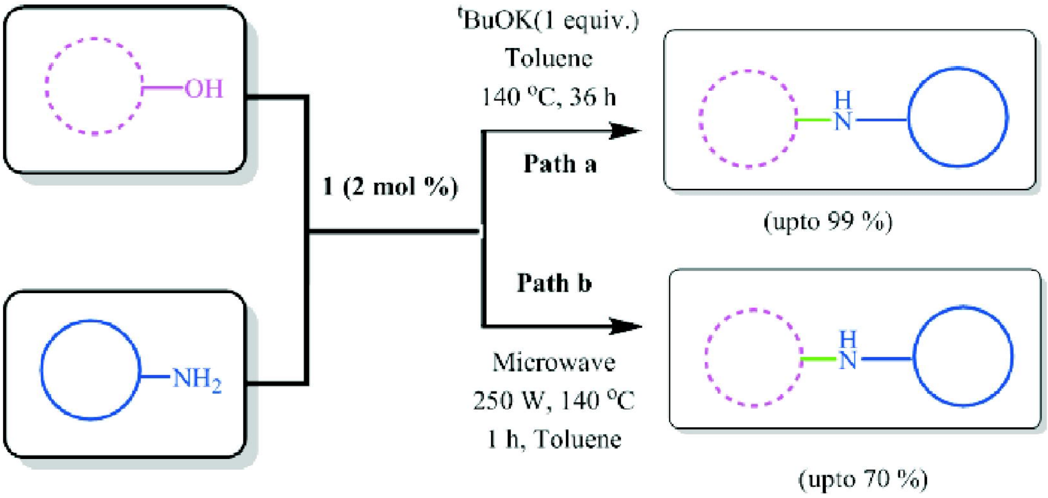
Contributory Paper-38

Catalysis in bimetallic Ni-Sn domain: Activation of Ar–NH_2, Ar–$CONH_2$, and sp^3-C–OH bonds

Mukesh Kumar Nayak and Sujit Roy*
Organometallics & Catalysis Laboratory,
School of Basic Sciences,
Indian Institute of Technology Bhubaneswar,
Argul, Khurda-752 050, Odisha
E-mail: sroy@iitbbs.ac.in
mk40@iitbbs.ac.in

Our laboratory has championed the concept of bimetallic catalysts in the Transition metal–Tin (TM-Sn) domain for the past two decades. All along our previous journey, the TM-partner belonged to late 4d- and 5d- elements[1–3].

The present work describes for the first time our successful entry into the 3d-TM–Sn domain using the catalyst (dppe)Ni$(SnCl_3)_2$ **1**[4]. Catalyst **1** showed excellent efficiency with lower catalyst loading (hence high TON) for the selective *N*-alkylation of aromatic and heteroaromatic amines and amides with alkyl and benzyl alcohols (Scheme 1). To the best of our knowledge, among the known nickel-based catalysts, **1** stands out distinctly by virtue of its TON and selectivity (Scheme 1, Path-a). Additionally, a base-free approach using **1** has been demonstrated under microwave irradiation (Scheme 1, Path-b).



Scheme 1. Activation of Ar–NH_2, Ar–$CONH_2$ and sp^3-C–OH Bonds in Presence of **1**.

In this presentation, the initial success, optimization, and scope of the reaction will be described in detail.

References

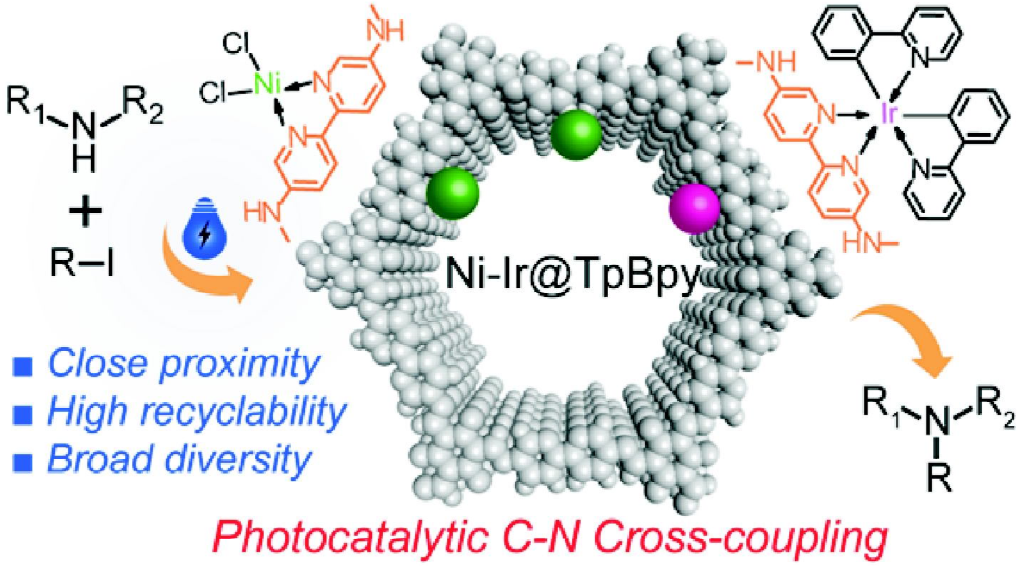
1. D. Das, S. S. Mohapatra and S. Roy, *Chem. Soc. Rev.*, 2015, **44**, 3666-3690.
2. J. Choudhury, S. Podder and S. Roy, *J. Am. Chem. Soc.*, 2005, **127**, 6162-6163.
3. P. Mukhi and S. Roy, *ChemistrySelect*, 2020, **5**, 1000-1006.
4. E. F. de Assis and C. A. L. Filgueiras, *Transit. Met. Chem.,* 1994, **191**, 1994, **19**, 78-80.

Contributory Paper-39

Dual metallation in a two-dimensional covalent organic framework for photocatalytic C–N cross-coupling reactions

Ayan Jati, Kaushik Dey, Maryam Nurhuda, Matthew A. Addicoat,
Rahul Banerjee* and Biplab Maji*
Department of Chemical Sciences,
Indian Institute of Science Education and Research Kolkata,
Kolkata
E-mail: aj19rs@35@iiserkol.ac.in
ayanjati@gmail.com

Covalent organic frameworks (COFs) are promising toolbox in the field of heterogeneous catalysis[1]. Herein, we report a dual metallation (iridium and nickel) strategy in a single 2D-COF TpBpy to perform a variety of C-N cross-coupling reactions[2]. Moving from the traditional approach[3], we focus on the COF-backbone as a host for metal catalysed photosensitive C-N coupling reactions. The controlled metallation and recyclability without deactivation of both catalytic centers are unique with respect to previously reported coupling strategies. We performed various photoluminescence and electrochemical studies with Hammett correlations to understand the mechanism. The developed protocol enables selective and reproducible coupling of a diverse range of amines (aryl, heteroaryl, alkyl), carbamide and sulfonamide with electron-rich, -neutral, and -poor (hetero)aryl iodides. Keeping this strategy in perspective, we explored the activity to produce non-steroidal anti-inflammatory drug Fulfenamic acid,



strong pharmacophore N,5-diphenyloxazol-2-amine, FDA approved drugs Flibenserin, Tripelennamine and did late-stage diversification of the derivatives of ibuprofen, naproxen, gemfibrozil, helional, glycine, and ε-aminocaproic acid.

References

1. A. P. Cote, A. I. Benin, N. W. Ockwig, M. O'Keeffe, A. J. Matzger and O. M. Yaghi, *Science,* 2005, **310**, 1166-70.
2. A. Jati, K. Dey, M. Nurhuda, M. A. Addicoat, R. Banerjee and B. Maji, *J. Am. Chem. Soc.*, 2022, **144**, 7822-7833.
3. S. Gisbertz, S. Reischauer and B. Pieber, *Nat. Catal*., 2020, **3**, 611-6.

Contributory Paper-40

A deoxygenation switch based red emitting fluorogenic light up probe for the detection of highly toxic free bilirubin in human blood serum

Ejaj Ahmed
The University of Burdwan,
Golapbag, Burdwan, West Bengal
E-mail: ahmmedchembu@gmail.com

Reaction-based chemical switches are attracting great interest due to their high selectivity, and their use has become a powerful technique for developing fluorogenic probes. Herein, a benzorhodol-derivative attached N-oxide probe (DEBNox) has been designed as a new fluorogenic probe for the detection of the biologically toxic species bilirubin based on a deoxygenation switching mechanism. Upon reaction with added Fe^{3+}, bilirubin produces Fe^{2+} ions *in situ*, which in turn promote a deoxygenation reaction with DEBNox to generate the corresponding high-red-fluorescence (λem: 623 nm) benzorhodol derivative (DEB). This type of Fe^{3+}-mediated response helps the probe to act as a qualified turn on selective fluorescence sensor for bilirubin with a detection range as low as 33 nM. Moreover, the probe was successfully employed to detect free bilirubin in human blood serum specimens with acceptable accuracy and reliability. This DEBNox-based light-up strategy also facilitates the construction of reliable and highly sensitive assays based on a paper-based strategy, similar to pH-indicator paper, as is demonstrated here via bilirubin detection in real serum samples. These findings could be useful for developing powerful diagnostic tools for the detection of free bilirubin in the near further.

Graphics:

Contributory Paper-41

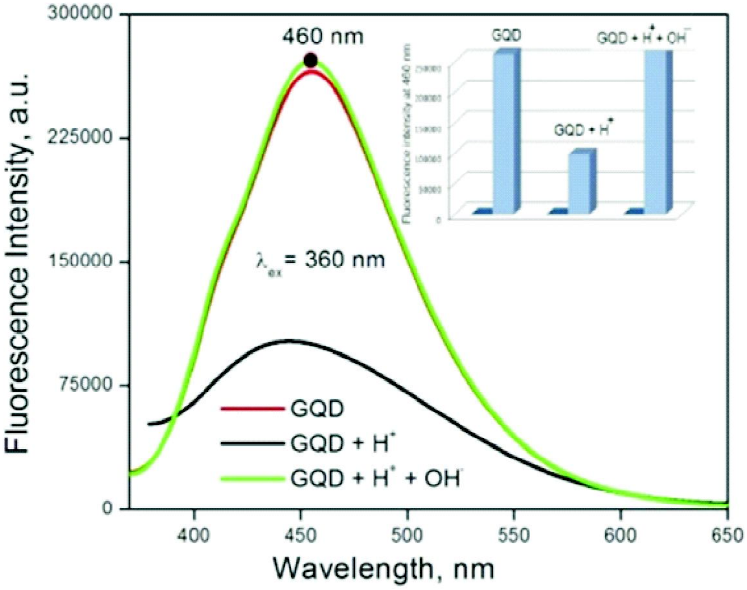
GQDs solution as molecular logic gates, memory element and a possible new password system

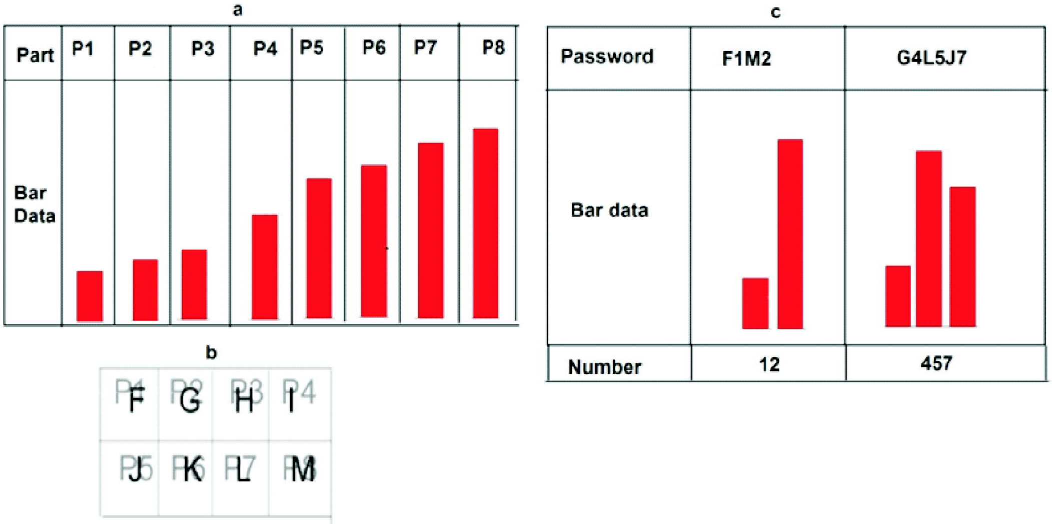
Pradip Shit and Asoke Prasun Chattopadhyay*
Department of Chemistry,
University of Kalyani,
Kalyani-741 235, Nadia
E-mail: asoke@klyuniv.ac.in

Graphene quantum dots (GQDs) synthesized in our laboratory are highly fluorescent (λabs 360 nm, λemiss 460 nm) and the fluorescence depends strongly on pH of the medium. On careful addition of H^+ and OH^- ions in the solution, fluorescence output at 460 nm can be made to behave as a binary switch. Suitable application of H^+ and OH^- inputs may lead to design of logic gates, and memory element with cyclic Erase-Read-Write-Read ability with set-reset feedback loop mechanism. Finally, pH depended fluorescence intensity at 460 nm can be utilized to produce highly secure combination of letters and numbers for an opto-chemical password system.

Reference

1. C. Y. Yao, H. Y. Lin, H. S. N. Crory and A. P. de Silva, *Mol. Syst. Des. Eng.*, 2020, **5**, 1325-1353.
2. M. P. Bhat, M. Kigga, H. Govindappa, P. Patil, H. Y. Jung, J. Yu and M. Kurkuri, *New J. Chem.*, 2019, **43**, 12734-12743.
3. U. Saha, M. Das, R. Dolai, J. Butcher and G. Suresh Kumar, *ACS Omega*, 2020, **5**, 18411-18423.
4. D. Pan, J. Zhang, Z. Li and M. Wu, *Adv. Mater.*, 2010, **22**, 734-738.
5. J. Dong, C. Shao, H. Chen, R. Li, Y. Wang, X. Lin Chi and G. Chen, *Carbon*, 2012, **50**, 4738-4743.


300000
225000
150000
75000
0
Fluorescence Intensity, a.u.
400
450
500
550
600
650
Wavelength, nm
460 nm
λ_{ex} = 360 nm
GQD
GQD + H$^+$
GQD + H$^+$ + OH$^-$
Fluorescence intensity at 460 nm
GQD
GQD + H$^+$
GQD + H$^+$ + OH$^-$


a
Part
P1
P2
P3
P4
P5
P6
P7
P8
Bar Data
b
P1 F
P2 G
P3 H
P4 I
P5 J
P6 K
P7 L
P8 M
c
Password
F1M2
G4L5J7
Bar data
Number
12
457

Contributory Paper-42

Zn(II) metal embedded 3D-COF (Zn@RIO-1) for synthesis of valuable products via CO_2 fixation under solvent free condition

Najirul Haque and Sk Manirul Islam*
Department of Chemistry,
University of Kalyani,
Kalyani, Nadia-741 235, West Bengal, India
E-mail: nazirulhaq95@gmail.com
manir65@rediffmail.com

Covalent organic frameworks (COFs) have been gaining substantial attentions over the past decade due to its emerging class of crystalline porous polymeric nature connected by vibrant covalent bonds and wide spread applications in various fields. Currently, three dimensional COFs (3D-COFs) are engaging spotlight due to their high surface area, unique porous features, and exceptional performances compared to formerly publish two dimensional (2D) frameworks with the AA-stacking layered mode. In this poster we are presenting a 3D-COF based zinc (II) catalyst (Zn@RIO-1), which is showing efficient chemical fixation of carbon dioxide to synthesize α-alkylidene cyclic carbonates and oxazolidinones from propargylic alcohols. The high surface area (312.61 m^2/g) containing microporous material facilitates both types of catalytic reactions under atmospheric CO_2 pressure. More importantly the easily recyclable and reusable catalyst produced moderate to high yield of desired carbonates as well as oxazolidinones products in solvent free condition. This study emphasizes the capability of 3D-COF based material in catalysis field, more specifically in the field of carbon dioxide capture and chemical fixation to fine chemicals. These results unlock the door to an entirely new class of protocol for chemical fixation of CO_2 into α-alkylidene cyclic carbonates and oxazolidinones from propargylic alcohols using 3D-COF as a potential heterogeneous ligand under sustainable conditions (i.e. solvent-free).

Reference

1. N. Haque, S. Biswas, S. Ghosh, A. H. Chowdhury, A. Khan, S. M. Islam, *ACS Applied Nano Materials,* 2021, **4(8)**, 7663-7674.
2. N. Haque, S. Biswas, P. Basu, I. H. Biswas, R. Khatun, S. M. Islam, *New J. Chem.*, 2020, **44**, 15446-15458.

Contributory Paper-43

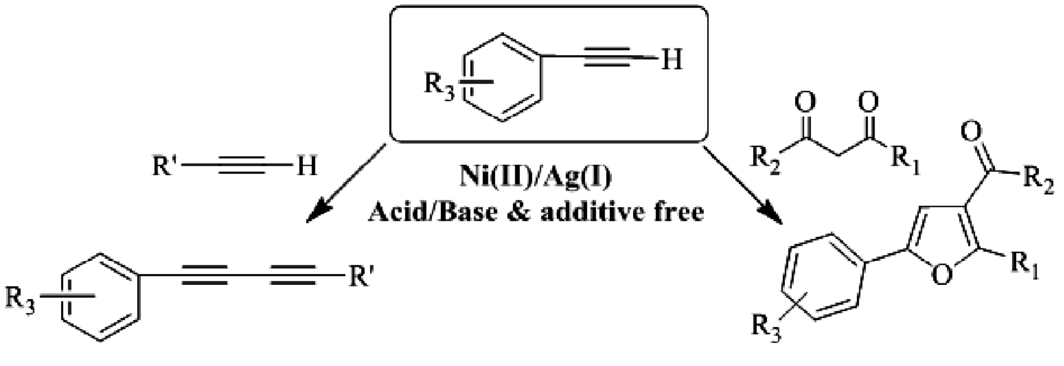
Ni(II)/Ag(I) dual metal catalysis towards sp^3 C-H functionalization: Novel routes to unsymmetrical diynes and furan

Anuradha Mohanty and Sujit Roy*
Organometallics & Catalysis Laboratory,
School of Basic Sciences,
Indian Institute of Technology Bhubaneswar,
Argul, Khurda-752 050, Odisha
E-mail: sroy@iitbbs.ac.in
am16@iitbbs.ac.in

C-H bond functionalization of terminal alkynes is one of the attractive and challenging approaches for the construction of direct C-C bond[1]. The past two decades have witnessed the emergence of multi-metallic catalysts (dual or single scaffold) in C-C bond forming reaction. When compared to their mono-metal counterpart, a multimetallic catalyst offers multi-prong design opportunity in directing the chemo-, regio- and stereo- selectivity in the product with high catalytic efficiency. A major program in our laboratory is in the area of heterobimetallic catalysis towards selective and atom-economic strategies for carbon-carbon and carbon-heteroatom bond formation[2]. In the present work[3,4], we introduce a novel Ni(II)/Ag(I) dual metal catalysis towards the following transformations (Scheme 1):

- A highly selective hetero-coupling of terminal alkynes.
- Tandem coupling of terminal alkynes for the synthesis of substituted furan.

Notably, the above reactions do not require acid, base, or additive and are highly atom-economic. The synthetic and mechanistic aspects of these transformations will be highlighted in the presentation.



Scheme 1

Reference

1. P. Siemsen, R. C. Livingston and F. Diederich, *Angew. Chem., Int. Ed.*, 2000, **39**, 2632.
2. D. Das, S. S. Mohapatra and S. Roy, *Chem. Soc. Rev.*, 2015, **44**, 3666.
3. A. Mohanty and S. Roy, *Chem. Commun.*, 2017, **53**, 10796.
4. A. Mohanty and S. Roy, *Eur. J. Org. Chem.*, 2019, **39**, 6702-6706.

Contributory Paper-44

Exploration of photoreduction ability of reduced graphene oxide–cadmium sulphide hetero-nanostructures

Bapan Bairy
The University of Burdwan,
Golapbag, Burdwan, West Bengal
E-mail: bapanbairy@gmail.com

Fabrication of effective photocatalyst using semiconductors and graphene or reduced graphene oxide has been regarded as one of the most promising task to attenuate the environmental pollution. This paper reports the synthesis of different nanocomposites of reduced graphene oxide–cadmium sulfide (RGO-CdS) with varying weight ratio of RGO by simple reflux condensation reaction, during which the reduction of graphene oxide (GO) and formation of CdS nanoparticles occur simultaneously. The combination of CdS nanoparticles (NPs) with the optimum amount of RGO gives a noticeable effect on the properties of the synthesized hybrid nanocomposites, such as enhanced optical, photocatalytic properties. The microscopic studies proved that with the increasing RGO content in the nanocomposites, the particle size decreases and got different shapes. These nanocomposites have been investigated separately as nanocatalyst for the reduction of Cr(VI) to Cr(III) in the presence of visible light irradiation and the catalytic activity depends on the pH of the medium and also the particle size of the CdS NPs which are supported by the band gap energy derived from Tauc's equation. The significant increase in photocatalytic performance of the RGO-CdS nanocomposite was attributed to high electron conductivity of the CdS NPs and RGO surface which facilitates charge separation and prolongs the lifetime of photogenerated electron–hole pairs by decreasing the recombination rate.

Contributory Paper-45

Light induced carboxylation of Aryl derivatives with cooperative COF as active photocatalyst and Ni(II) co-catalyst

Pekham Chakrabortty and Sk. Manirul Islam*
Department of Chemistry,
University of Kalyani,
Kalyani, Nadia-741 235, West Bengal, India
E-mail: pekhamchakrabortty55@gmail.com
manir65@rediffmail.com

Catalysis plays a significant role in the growing demand for industrial processes. Photocatalytic carboxylation of Aryl derivatives was demonstrated under the atmospheric pressure of CO_2 using the mesoporous Covalent Organic Framework (COF) as the active photocatalyst under visible light[1]. Application of covalent organic framework-based catalysts in carbon dioxide fixation reactions has been received attention in recent years due to their potential advantages over the homogeneous ones[2,3]. The present work consists of synthesis, characterization and catalytic evaluation of different porous materials-based catalysts and their applications in CO_2 fixation reactions. These catalysts have been characterized by powder XRD, TEM, EDX, FT-IR, EPR, BET, XPS, SEM-EDX, UV-Vis spectral studies and thermo gravimetric analysis.

Good catalytic activity and efficiency of these catalysts in the carbon dioxide fixation reaction suggest that the present catalytic systems would be useful to synthesize industrially important fine chemicals.

Reference

1. P. Chakrabortty, A. Das, A. H. Chowdhury, S. Ghosh, A. Khan and S. M. Islam, *New Journal of Chemistry*, 2021, **45**, 4738-4745.
2. S. Ghosh, R. A. Molla, U. Kayal, A. Bhaumik and S. M. Islam, *Dalton Transaction,* 2019, **48**, 4657-4666.
3. M. Halder, Md. M. Islam, Z. Ansari, S. Ahammed, K. Sen and S. M. Islam, *ACS Sustainable Chemistry &* Engineering*,* 2017, **5**, 648.

Contributory Paper-46

Detailed investigation on oppositely charged polyelectrolyte-surfactant

Sourav Das and Soumen Ghosh*
Centre for Surface Science,
Department of Chemistry,
Jadavpur University,
Kolkata-700 032, India
E-mail: subhapresi@gmail.com

Investigation has been made on the interaction of a biodegradable anionic polyelectrolyte, sodium alginate (NaAlg) with two oppositely charged cationic surfactants, 1-hexadecyl-3-methyl imidazolium chloride (C_{16}MImCl) and 1-hexadecyl triphenylphosphonium bromide (C_{16}TPB), former is a Surface-Active Ionic Liquid (SAIL) and latter a conventional surfactant over a wide concentration regime of polyelectrolyte. Dual influence of electrostatic and hydrophobic interactions plays in this investigation when mixing surfactants to oppositely charged polyelectrolyte. A number of different experimental techniques, e.g., conductometry, tensiometry, steady state and time resolved spectrofluorimetry, turbidimetry, isothermal titration calorimetry (ITC), dynamic light scattering (DLS), attenuated total reflection (ATR), high resolution transmission electron microscopy (HR-TEM) and fluorescence microscopy have been implemented to get comprehensive information originated from the interaction of oppositely charged polyelectrolyte and surfactants. Irreversible phase separation of oppositely charged polyelectrolyte- surfactant complex (PS-complex) occurs at higher polyelectrolyte concentration investigated here for both the surfactants. Study of oppositely charged polyelectrolyte in conjugation with surfactants generate new field of opportunities and have been used in multifaceted industrial formulations, in detergents, emulsions, waste-water treatment, oil-recovery and more.

References

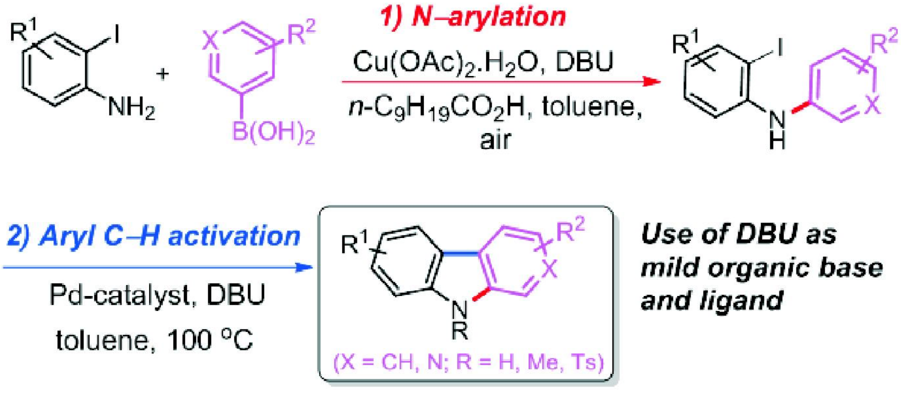
1. A detailed assessment on the interaction of sodium alginate with a surface-active ionicliquid and a conventional surfactant: A multitechnique approach; S. Das and S. Ghosh, *Phys. Chem. Chem. Phys.,* 2022, **24**, 13738-13762.
2. Intermolecular interactions in polyelectrolyte and surfactant complexes in solution; N. Khan and B. Brettmann, *Polymers*, 2018, **11**, 51.
3. Adsorption of oppositely charged polyelectrolyte/surfactant mixtures. Neutron reflection from alkyl trimethylammonium bromides and sodium poly (styrene sulfonate) at the air/water interface: The effect of surfactant chain length; D. J. Taylor, R. K. Thomas, P. X. Li and J. Penfold, *Langmuir,* 2003, **19**, 3712-3719.

Contributory Paper-47

Efficient synthesis of nitrogen containing fused heterocyclic compounds involving Pd/DBU-catalyzed coupling reactions

Aminur Khan, Rejaul Karim and Safiul Alam*
Department of Chemistry,
Aliah University, IIA/27, New Town,
Kolkata-700 160, India
E-mail: khanrph92@gmail.com
safiul_ku@yahoo.co.in

Practical access to diversely functionalized carbazoles has been developed by consecutive Cu-catalyzed Chan-Lam *N*-arylation of various *o*-iodoanilines and boronic acids, and Pd-catalyzed intramolecular aryl C-H activation of 2-iodo-*N*-arylanilines. Use of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) as base was found beneficial for both steps. In the Pd-catalyzed C-H activation step, DBU acts as ligand as well as base, resulting in improved functional tolerance and higher yields than those observed with inorganic or other nitrogen bases. This DBU-assisted sequence offers access to a variety of carbazoles with various electron-donating and electron-withdrawing substituents, including halogens or other reactive functional groups. Twenty-eight cabazoles with various substitution patterns, including two naturally-occurring carbazoles-clausine L and clausine H - have been successfully synthesized using these DBU- promoted metal-catalyzed coupling reactions.



References

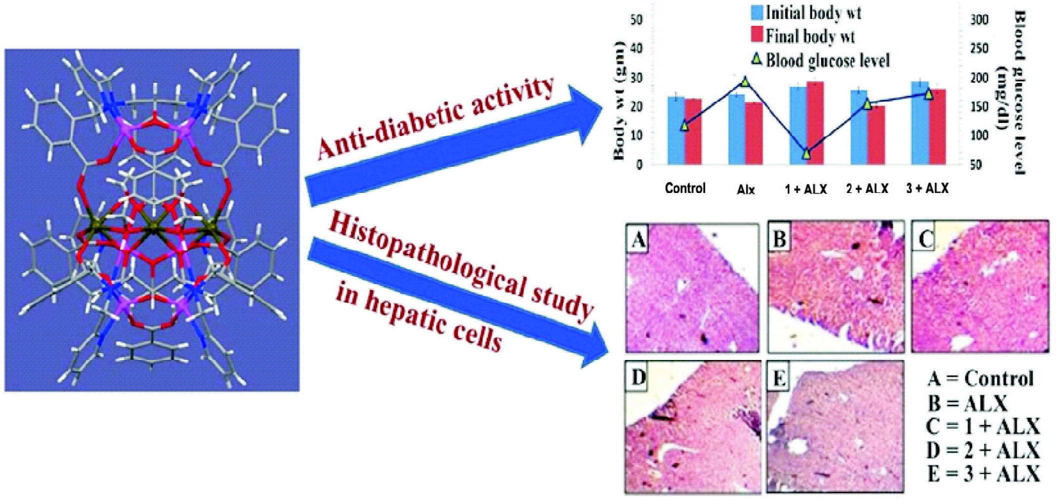
1. (a) T. W. Lynos and M. S. Sanford, *Chem. Rev.,* 2010, **110**, 1147;
   (b) X. Chen, K. M. Engle, D.-H. Wang and J.-Q. Yu, *Angew. Chem. Int. Ed.,* 2009, **48**, 5094.
2. R. R. Bedford and C. S. J. Cazin, *Chem. Commun.,* 2002, 2310.
3. D. Tsvelikhovsky and S. L. Buchwald, *J. Am. Chem. Soc.,* 2010, **132**, 14048.
4. A. Khan, R. Karim, H. Dhimane and S. Alam, *ChemistrySelect.,* 2019, **4**, 6598.

Contributory Paper-48

Carboxylate bridge-supported assembly of $[Zn_2]$ building units leading to the formation of $[Zn_6]$ complexes: Synthesis, structure and biological studies

Avishek Majumder, Nityananda Dutta and Manindranath Bera*
Department of Chemistry,
University of Kalyani,
Kalyani-741 235, West Bengal, India
E-mail: mbera2009@klyuniv.ac.in

A new family of $[Zn_6]$ complexes $[Na_3Zn_6(cpdp)_3(\mu\text{-}Bz)_3(CH_3OH)_6][ZnCl_4][ZnCl_3(H_2O)]\cdot3CH_3OH\cdot1.5\ H_2O$ (**1**), $[Na_3Zn_6(cpdp)_3(\mu\text{-}p\text{-}OBz)_3(CH_3OH)_6]\cdot2H_2O$ (**2**) and $[Na_3Zn_6(cpdp)_3(\mu\text{-}p\text{-}NO_2Bz)_3(CH_3OH)_6]Cl_3\cdot2H_2O$ (**3**), supported by carboxylate-based multidentate ligand, *N*,*N′*-bis[2-carboxybenzomethyl]-*N*,*N′*-bis[2-pyridylmethyl]-1,3-diaminopropan-2-ol (H_3cpdp) have been synthesized and characterized [Bz = benzoate; *p*-OBz = dianion of *para*-hydroxybenzoic acid; *p*-NO_2Bz = *para*-nitrobenzoate]. The molecular structures of **1-3** have been determined by single crystal X-ray crystallography. In solution, the UV-Vis and NMR spectroscopic data establish the 1:2 composition of the $(cpdp^{3-})_3/(Zn^{2+})_6$ in **1-3**. Meticulous biological studies performed in mice model suggested the possible anti-diabetic efficacy and anti-cancer activities of the complexes. Experimental results indicated that **1** seems to be a better compound for overall diabetic management and control, whereas **2** and **3** seem to be the promising compounds for designing chemo-preventive drugs against the hepatic carcinoma.



References

1. A. Patra, T. K. Sen, A. Ghorai, G. T. Musie, S. K. Mandal, U. Ghosh and M. Bera, *Inorg. Chem.*, 2013, **52**, 2880-2890.
2. A. Patra, S. K. Saha, T. K. Sen, L. Carrella, G. T. Musie, A. R. Khuda-Bukhsh and M. Bera, *Eur. J. Inorg. Chem.*, 2014, 5217-5232.
3. N. Dutta, S. Haldar, G. Vijaykumar, S. Paul, A. P. Chattopadhyay, L. Carrella and M. Bera, *Inorg. Chem.*, 2018, **57**, 10802-10820.
4. A. Majumder, N. Dutta, S. Dey, P. Sow, A. Samadder, G. Vijaykumar, K. Rangan and M. Bera, *Inorg. Chem.*, 2021, **60**, 17608-17626.

Contributory Paper-49

Construction of block copolymer and amino acid based ABS: An efficient extraction tool for PPI

Laboni Das and Kamalika Sen*
Department of Chemistry,
University of Calcutta,
92 Acharaya Prafulla Chandra Road,
Kolkata-700 009, India
E-mail: kamalchem.roy@gmail.com

Aiming to construct a biocompatible aqueous biphasic system (ABS), amino acids and block copolymer based ABSs have been designed. Glycine and L-proline can successfully salt out PPG-PEG-PPG block copolymer and can form the biphase even in room temperature. Whereas L-alanine requires at least 318 K under normal atmospheric pressure to create the ABS with block copolymer. The phase diagrams for all the systems have been constructed using turbidometric method at different temperatures and the corresponding binodal graphs are plotted with the help of Merchuk equation[1]. An increase in temperature leads to an increase in biphasic region. Tie line lengths, slope of tie line lengths and the compositions of both the phases of the corresponding ABSs have been determined using the gravimetric method[2]. The presence of amino acids in the place of ionic salts as one of the phase forming component, makes the ABS eligible to extract medically relevant molecules. Herein, the proton pump inhibitors (PPIs), 'one of the most prescribed medicines in the world', are extracted using the newly designed amino acid and block copolymer based ABSs. The complete extractions of Rabeprazole and Pantoprazole were achieved by glycine based ABS, whereas ~83% of Esomeprazole was extracted by the same. The extraction efficacy of the other two amino acid based ABSs are also noticeable.

References

1. K. Sen, A. Chakraborty, A glycine based aqueous biphasic system: Application in sequential separation of Ni, Cu and Zn. *J. Mol. Liq.*, 2016, **218**, 106-111.
2. J. C. Merchuk, B. A. Andrews and J. A. Asenjo, Aqueous two-phase systems for protein separation: Studies on phase inversion. *J. Chromatogr., Biomed. Appl.*, 1998, **711**, 285-293.

Contributory Paper-50

Encapsulation of a dietary polyphenol in β-casein micelles: Interactions and effect on bioactivity

Priti Sengupta[a,b], Adity Bose*[b] and Kamalika Sen*[a]
[a]Department of Chemistry,
University of Calcutta,
92, Acharaya Prafulla Chandra Road,
Kolkata-700 009, India
[b]Department of Chemistry,
Presidency University,
86/1 College Street,
Kolkata-700 073, India
E-mail: pritisengupta1@gmail.com

Dietary polyphenols are secondary metabolites of plants with a wide range of unique bioactive qualities, making them highly valued for their positive impacts on human health and well-being. Several factors like poor water solubility, instability in GI tract, etc., limits their practical applications by suppressing their functional abilities and bioaccessibility. Encapsulation of polyphenols in appropriate nanocarriers is the most popular approach taken by researchers to address the aforementioned problems. Carrier systems based on food proteins hold much potential due to their excellent biocompatibility and biodegradability. Milk proteins are an excellent available choice for researchers in this respect. β-casein (βCN) comprises of ~36–40% of the bovine milk caseins and are extensively used for multipurpose application. Due to the presence of hydrophobic C-terminal domain and hydrophilic N-terminal domain, βCN self-assembles into stable micellar structures in aqueous solution under physiological conditions.

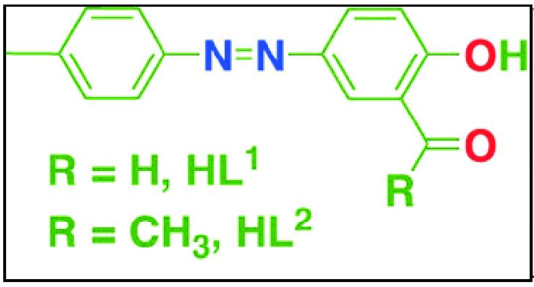
In the present work, we have chosen rutin (a flavonol glycoside) as polyphenol. Rutin is well recognized for its potential antioxidant, antidiabetic, antitumor and other biological activities. The binding interactions of rutin with βCN has been explored using different spectroscopic tools. Also, the effect of encapsulation on the bioactivity of rutin, particularly antioxidant activity, *in vitro* release (in simulated gastric and intestinal fluids) profile and bioaccessibility, have been considered. Keeping in mind, the low aqueous solubility of rutin leading to multiple-dosage regimen problems, sustained release kinetics is sought after. The present work aids in the development of casein-based sustained delivery systems of polyphenols by providing more insight into the rutin-βCN interaction processes.

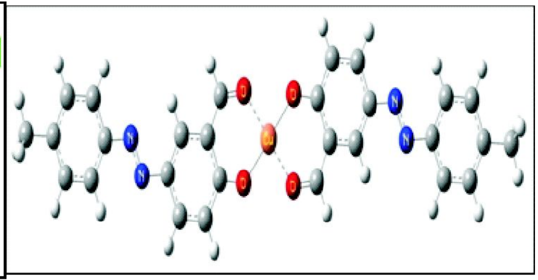
Contributory Paper-51

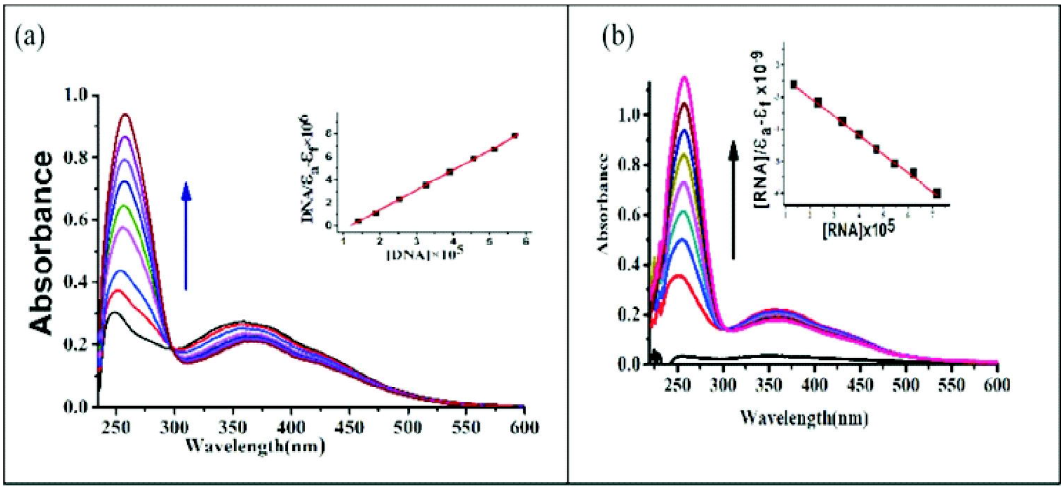
Copper(II)- complexes of azo based ligands; 2-hydroxy-5-*p*-tolylazo-benzaldehyde and 1-(2-hydroxy-5-*p*-tolylazo-phenyl)-ethan-one: Synthesis, structure, spectra, nucleic acid binding and molecular docking studies

Gourisankar Roymahapatra*[a], Mamta Tripathi[b] Mrinal Kanti Dash[a]
and Avijit Sarkar[c]
[a]Department of Applied Science,
Haldia Institute of Technology,
Haldia-721 657, India
[b]School of Studies in Chemistry,
Pt. Ravishankar Shukla University,
Raipur-492 010, India
[c]Department of Chemistry,
Bhairab Ganguly College, Belghoria,
Kolkata-700 056, India
E-mail: gourisankar1978@gmail.com

Two new Copper(II)- complexes were synthesized from azo-based ligands 2-hydroxy-5-p-tolylazo-benzaldehyde (**L1**) and 1-(2-hydroxy-5-p-tolylazo-phenyl)-ethan-one (**L2**). The ligands and their corresponding Cu(II)-complexes-[Cu(L_1)$_2$] (**1**) and [Cu(L_2)$_2$] (**2**) were characterized by elemental analysis, NMR (^{1}H and ^{13}C) analysis, IR and UV/Vis spectroscopic techniques. Spectroscopy and theoretical optimization studies reveal the geometry of copper complexes. Both the complexes were tested for drug-likeliness molecules by investigating their binding behavior with nucleic acids (DNA/RNA). All the synthesized complexes were checked for their applicability as nucleic acid binders. Experimentation findings followed by computation exploration predict specific binding interaction of complexes at a specific region of DNA and RNA. The experimental finding along with computational analysis concludes electrostatic binding via partial groove as the mode of binding. [Cu(L_1)$_2$] (**1**) and [Cu(L_2)$_2$] (**2**)







both complexes show potency as drug-like molecules, and outcomes successfully support them for further screening.

Reference

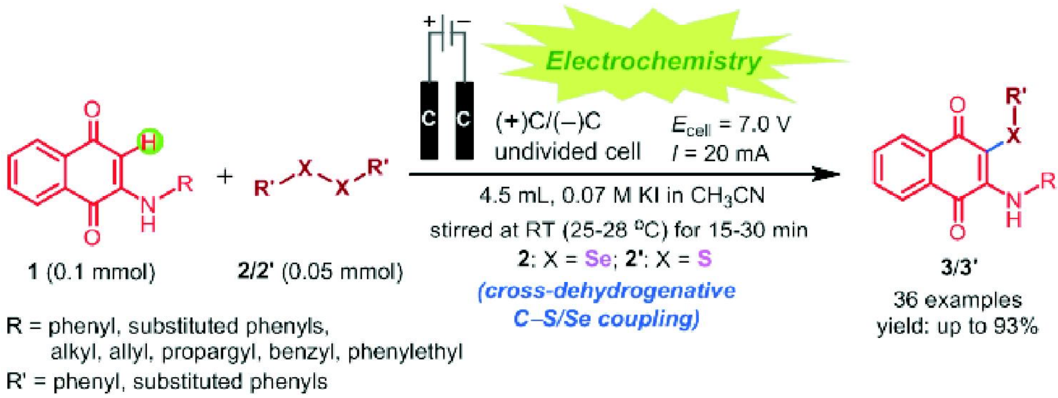
1. *Open Chemistry,* 2022, **20**, 505-516. https://doi.org/10.1515/chem-2022-0164.

Contributory Paper-52

Electrochemical regioselective C(sp^2)-H selenylation and sulfenylation of substituted 2-amino-1,4-naphthaquinones

Pintu Karmakar, Debopam Pal, Suravi Das and Goutam Brahmachari*
Laboratory of Natural Products & Organic Synthesis,
Department of Chemistry,
Visva-Bharati (a Central University),
Santiniketan-731 235, West Bengal, India
E-mail: goutam.brahmachari@visva-bhartai.ac.in

The application of electrochemical strategy has recently emerged as a hot research topic in synthetic methodology. This technique has already offered an effective alternative to conventional methods in oxidative C–H functionalization reactions. We have now successfully unearthed an electrochemical strategy as an alternative method for accessing the 2,3-thioaminated version of 1,4-naphthoquinones along with a new series of 2,3-selenoaminated analogs. The process involves regioselective C(sp^2)-H selenylation and sulfenylation of substituted 2-amino-1,4-naphthaquinones (**1**) *via* oxidative *cross*-coupling between the substrates **1** and diversely substituted diselenides (**2**)/disulfides (**2′**) in an electrochemical cell using KI as the electrolyte in acetonitrile at ambient temperature. This oxidative *cross*-coupling reaction avoids the use of transition metal catalysts, additives, oxidants and high temperatures. The other notable advantages of this protocol are the tolerance of diverse functional groups, mild reaction conditions at ambient temperature, energy-efficiency, good to excellent yields, short reaction times (in minutes), gram-scale applicability, and eco-friendliness.



Scheme 1. Electrochemical synthesis of 3-selenylated/sulfenylated derivatives of 2-amino-1,4-naphthaquinones.

References

1. I. Karmakar and G. Brahmachari, *Green Chem.*, 2022, **24**, 2825-2838.
2. M. Mandal and G. Brahmachari, *J. Org. Chem.*, 2022, **87**, 4777-4787.
3. N. Nayek, P. Karmakar, M. Mandal, I. Karmakar and G. Brahmachari, *New J. Chem.*, 2022, **46**, 13483-13497.
4. G. Brahmachari, I. Karmakar and P. Karmakar, *Green Chem.*, 2021, **23**, 4762-4770.
5. G. Brahmachari and I. Karmakar, *J. Org. Chem.*, 2020, **85**, 8851-8864.

Contributory Paper-53

Structural elucidation, DFT calculations and catalytic activity of dioxomolybdenum(VI) complexes with N,N donor ligand: Role of halogen atom coordinated to the molybdenum centre

Malini Roy[a], Debanjana Biswal[a], Nikhil Ranjan Pramanik*[b], Michael G. B. Drew[c], Suvendu Paul[d], Payal Kachhap[e], Chanchal Haldar[e], Syamal Chakrabarti*[a]
[a]Department of Chemistry,
University College of Science,
92, Acharya Prafulla Chandra Road,
Kolkata-700 009, West Bengal, India
[b]Department of Chemistry,
Bidhannagar College, EB-2, Sector-1, Salt Lake,
Kolkata-700 064, India
[c]Department of Chemistry,
The University of Reading, Whiteknights,
Reading RG6 6AD, UK
[d]Department of Chemistry, University of Kalyani,
Kalyani, Nadia-741 235, West Bengal, India
[e]Department of Applied Chemistry,
Indian Institute of Technology (ISM), Dhanbad,
Dhanbad-826 004, Jharkhand, India
E-mail: roymalini1992@gmail.com

Two new isostructural mononuclear dioxomolybdenum(VI) complexes of the formula MoO_2X_2L [where, X = Cl (**1**), Br (**2**)] are synthesized with a N,N donor 2-(3-methyl-5-phenyl pyrazol-1-yl) benzthiazole ligand (L). The complexes **1** and **2** are prepared by refluxing the parent $MoOX_3L$ in dichloromethane medium by aerial oxidation. The complexes are characterized by a wide range of spectroscopic techniques (IR, UV-Vis and ^1H NMR) and elemental analyses. Crystal structures of the ligand and complexes **1** and **2** are determined by single crystal X-ray diffraction which reveals a distorted octahedral geometry around the molybdenum(VI) centre in both the complexes. The ligand and the complexes build up fascinating supramolecular assembly *via* several non-covalent interactions including hydrogen bonding, $C\text{-}H\cdots\pi$ and $\pi\cdots\pi$ interactions. Further, a detailed study of Hirshfeld surface analysis and fingerprint plots of complex **1** and **2** are presented for understanding the intermolecular interactions involved in building self-assembled frameworks. Supportive DFT and TD-DFT calculations are also carried out. Electrochemical properties of the complexes are examined by cyclic voltammetry. Catalytic performance of the synthesized complexes is evaluated for the oxidation of different olefins in the presence of hydrogen peroxide.

Contributory Paper-54

Removal of chromium from an aqueous solution by using activated charcoal of neem leaves, neem bark and sweet lime peel

Naresh Giri and Pallavi Mishra*
Department of Chemistry,
J.N.V. University,
Jodhpur-342 001, Rajasthan
E-mail: pallavianuk@gmail.com

Industrial Water pollution from Industries is a potential threat to human health mainly because of the non-biodegradable, hazardous heavy metals. Among these heavy metals, Chromium is of considerable concern. Various methods adopted to remove heavy metals include chemical precipitation, membrane separation, ion exchange and adsorption. In the case of adsorption, the generally used adsorbents like activated carbon, silica, alumina, etc., are expensive. This has prompted using natural materials as adsorbents to develop cheaper alternatives, which can be disposed of without regeneration due to their lower cost. And so, Neem leaves, Neem bark and Sweet lime peel were tried for the removal of Chromium. The newly developed adsorbents should be as effective as (or more than) the conventional ones. Hence, in the present work, activated charcoal of Neem leaves, bark, and sweet lime peel is used to remove Chromium from aqueous solutions. The equilibrium studies were systematically carried out in a batch process covering various process parameters, including agitation time, adsorbent dosage, initial concentration of Chromium, the volume of an aqueous solution and pH of an aqueous solution. Adsorption behaviour was found to follow Freundlich's Adsorption Isotherm in the case of all adsorbents. Still, the Neem leaves powder was proved to be more promising than other Charcoal in removing Chromium.

Contributory Paper-55

Assessment of heavy metals concentration due to use of effluent water in the agricultural fields of Western Rajasthan

Pooja Prajapati and Pallavi Mishra
Department of Chemistry,
J. N. V. University,
Jodhpur-342 001, Rajasthan
E-mail: pallavianuk@gmail.com

Western Rajasthan is known for the scarcity of water and farmers are using readily available, untreated industrial effluent and sewage water for irrigation. There are a lot of textiles, steel, handicraft, glass, printing industries present in this area. They discharge their effluents without any treatment in to the canals and water bodies. As a result, these water bodies have become highly polluted. The objective of our study was to analyze the heavy metal contents in the vegetables and food grains, which are grown in the agricultural fields of Jodhpur especially near Jojari river area. Our selected study areas were Basni, Dangiyawas, Sangaria, Salawas and Vinayikiya where maximum use of effluent water for irrigation is observed. We collected various vegetables, cereal, pulses and millet samples grown in this area. We have analyzed the concentration of Cd, Cr, Pb and Cu in these samples after digestion with the help of AAS. In our studies alarmingly high concentration of heavy metals in the cereals, millets and pulses were observed. Concentration of lead and cadmium were found to be way above permissible limits. Consumption of such cereals and millet is very dangerous for human and animal health.

Contributory Paper-56

Kinetics and mechanism of oxidation of formic and oxalic acids by benzimidazolium fluorochromate

Jitendra Ojha and Pallavi Mishra*
Department of Chemistry,
J. N. V. University,
Jodhpur-342 001, India
E-mail: jitendraojha081089@icloud.com

Benzimidazolium fluorochromate(BIFC) is a mild oxidizing agent and we have used it for the specific oxidation of formic and oxalic acid in the dimethyl sulphoxide solution. Corresponding carbon dioxide were the products obtained after oxidation. The reaction was first order both in BIFC and the formic and oxalic acid. All kinetic studies were done using P-toluene sulphonic acid as catalyst was used for our reactions. Different organic solvents were used to study the reaction kinetics. Multi-parametric equations were used to study solvent effect. Suitable mechanism has also been suggested.

Contributory Paper-57

Different Hydrogen (H_2) storage methods and possibilities; a brief review

Surya Kanta Giri*[a] and G. Roymahapatra[b]
[a]Department of Applied Science,
[b]Department of Chemical Engineering,
Haldia Institute of Technology,
Haldia-721 657, India
E-mail: suryagiri064.hitche2020@gmail.com
grm.chem@gmail.com

Green energy, green fuel, hydrogen fuel and hydrogen economy.... are the buzzwords over the last two decades. The first element of the periodic table has become a global concern, this is because; the diatomic gas molecule has the potential to address the challenges in the global mission to achieve 'Net Zero emissions' by 2050. Hydrogen (H_2) exhibits the highest heating value per mass of all chemical fuels; it is regenerative and environmentally friendly.

But storing of H_2 is a hard job. Till date, H_2 can be stored using six different methods and phenomena: (i) high-pressure gas cylinders, (ii) liquid hydrogen in cryogenic tanks, (iii) adsorbed hydrogen on materials with a large specific surface area, (iv) absorbed on interstitial sites in a host metal (at ambient pressure and temperature), (v) chemically bonded in covalent and ionic compounds (at ambient pressure), or (vi) through oxidation of reactive metals, e.g. Li, Na, Mg, Al, Zn etc..

In this project paper we have reviewed different methods and possibilities, which will help to new researcher to choose their own objective of research.

Contributory Paper-58

Inhibition of Amyloid Fibril formation of human insulin by effective metal ions

Swarnali Paul and Umesh Chandra Halder*
Department of Chemistry,
Jadavpur University
Kolkata-700 032, India
E-mail: uhalder2002@yahoo.com

Human Insulin can form aggregates (nonnative cross-β-sheet rich fibrous structures i.e., amyloid fibril) due to its aggregation-prone properties at the site of repeated injection of type II diabetic patients and during *in vitro* storage condition. Neurodegenerative diseases and amyloidosis are closely related. Human insulin is a widely used model protein for the study of amyloid formation and inhibition as its fibrillary nature resembles that of other amyloid prone proteins like Amyloid precursor protein (Aβ peptides causing Alzheimer's disease), Atrial natriuretic factor (Amyloid ANF causing Atrial amyloidosis), and Prion protein (causing Spongiform encephalopathies) etc. To counteract this process, polypeptides, flavonoids were employed but with limited scope.

In this study, human insulin amyloid formation *in vitro* & whether metal ions can restrict this aggregation process of insulin under our experimental condition is studied. A combined biophysical, multi-spectroscopic, light scattering studies, electron microscopic studies and molecular docking experiments have been employed to understand the mechanism of inhibitions of the metal ions with the protein and investigation of the kinetics of prevention of insulin amyloid fibrillar structure formation is done. It revealed that two d-block metal-ions [Cu (II) and Fe(III)] can prevent the aggregation of it at very minute concentrations, one of them can even stabilize the native conformation of insulin when incubated at specific ratio. In this study, the possible mechanism of such inhibition have been proposed in terms free energy changes during the said metal-protein interaction. Metal ions are very interactive towards complex formation with protein structure and being micronutrients they are less toxic too. So, this study might be helpful in designing anti-amyloid therapeutics agents during *in vivo* studies also.

Contributory Paper-59

Phosphate sensing using a mixed-metal MOF

Sayani Hui and Partha Mahata*
Department of Chemistry,
Jadavpur University,
Kolkata-700 032, India
E-mail: sayanihui@gmail.com

A two - dimensional heterobimetallic luminescent metal-organic framework, $[YMn_{1.5}(C_7N_1H_3O_5)_3(H_2O)_6]\cdot 11H_2O$, **1** {where $C_7N_1H_3O_5$ = chelidamate}, was successfully synthesized by hydrothermal technique using chelidamic acid, Y(III) and Mn(II) ions. Single-crystal X-ray diffraction analysis of **1** indicates a two- dimensional structure with phenolic hydroxyl functionalized pockets. The phase purity of compound **1** was confirmed by powder X-ray diffraction. Compound **1** was systematically characterized *via* TGA, IR, UV-Vis spectroscopy. The compound **1** shows excellent photoluminescence through the excitation of 280 nm light. The emission of compound **1** was utilized for the selective detection of the phosphate anion in the aqueous medium by luminescence turn-on. The main reason behind the luminescence enhancement of compound **1** in presence of very minute concentration of the above-mentioned anion lies based on Bronsted-Lowry acid-base interactions. Phosphates (PO_4^{3-}) entered the hydroxyl functionalized pockets of **1** and stabilized the aromatic part of the MOF through molecular level interactions *via* the acid-base interactions. These interactions enhanced the luminescence intensity by reducing non-radiative transitions. Time-correlated single photon counting (TCSPC) measurement studies also proved the luminescent enhancement phenomenon of phosphate (PO_4^{3-}) by increasing the excited state lifetime with the increase of concentration of phosphate anions. The observed limit of detection (LOD) was 0.321 μM (30.49 ppb) for phosphate (PO_4^{3-}) and the observed luminescence enhancement coefficient, K_{SV} value was supreme to those of all other metal- organic frameworks reported previously. More importantly, the LOD value is significantly lesser than the recommended level for this anion towards human body.

Contributory Paper-60

Geometric brownian information engine: Upper bound of the achievable work under feedback control

Syed Yunus Ali*, Rafna Rafeek and Debasish Mondal
Department of Chemistry and Center for Molecular and
Optical Sciences & Technologies,
Indian Institute of Technology Tirupati,
Yerpedu-517 619, Andhra Pradesh, India
E-mail: cy18d503@iittp.ac.im

We design a geometric Brownian information engine by considering over-damped Brownian particles inside a two-dimensional monolobal confinement with irregular width along the transport direction. Under such detention, particles experience an effective entropic potential which has a logarithmic form. We employ a feedback control protocol as an outcome of error-free position measurement[1]. The protocol comprises three stages: measurement, feedback and relaxation. We reposition the center of the confinement to the measurement distance x_p instantaneously when the position of the trapped particle crosses x_p for the first

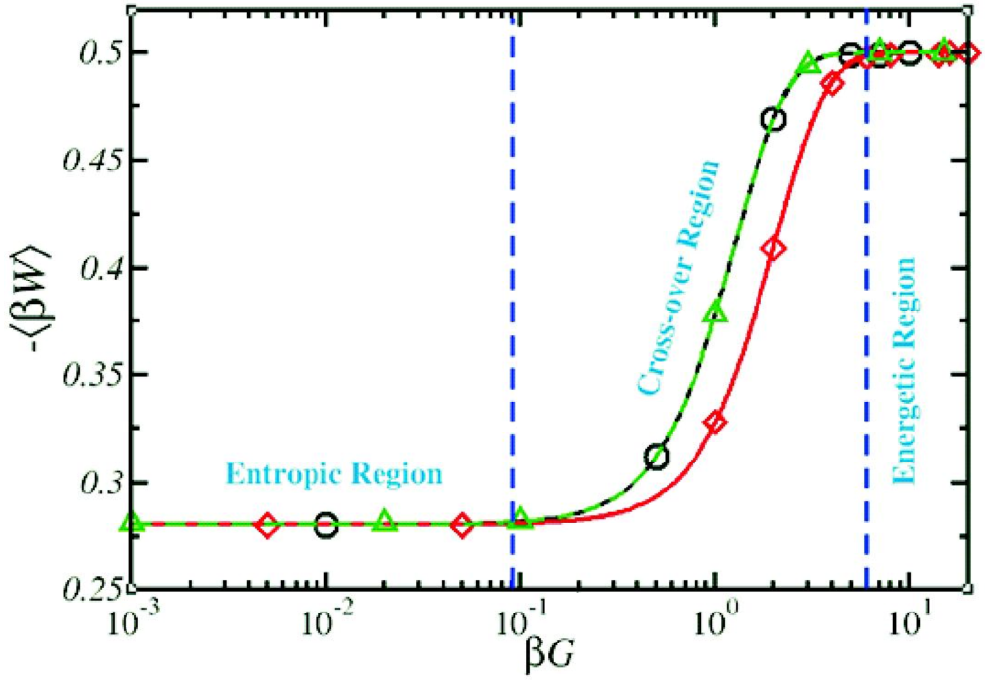


Fig. 1. Variation of extracted work with $\frac{G}{D}$ for different confinement parameters.

time. Then, the particle is allowed to thermal relaxation. We calculate the extractable work, total information and unavailable information associated with the feedback control using this equilibrium probability distribution function. We find the exact analytical value of the upper bound of extractable work as $\left(\frac{5}{3} - 2ln2\right)k_BT$ [2]. We introduce a constant force G downwards to the transverse coordinate (y). A change in G alters the effective potential of the system and tunes the relative dominance of entropic and energetic contributions in it. The upper bound of the achievable work shows a cross-over from $\left(\frac{5}{3} - 2ln2\right)k_BT$ to $\frac{k_BT}{2}$ when the system changes from an entropy dominated regime to energy dominated one[2]. Compared to an energetic analogue, the loss of information during the relaxation process is higher in the entropy-dominated region, which accredits the less value in achievable work. Theoretical predictions are in good agreement with the Langevin dynamics simulation studies.

References

1. Y. Ashida, K. Funo, Y. Murashita and M. Ueda, *Phys. Rev. E*, 2014, **90**, 052125.
2. S. Y. Ali, R. Rafeek and D. Mondal, *J. Chem. Phys.*, 2022, **156**, 014902.

Contributory Paper-61

Oxidataion of thiols by metal coordinated superoxide in acidic media

Ritu Mukherjee*
Department of Chemistry,
Dum Dum Motijheel College,
Kolkata-700 074
E-mail: ritu069@gmail.com

In weakly acidic media ($[H^+]$, 0.01–0.06 *M*), 2-mercaptoethanol (mercap, RSH), thioglycolic acid (tga, R′SH) and reduce the superoxo ligand of the complex ion, $[(en)_2(NH_3)CoO_2Co(en)_2(NH_3)]^{5+}$(**1**) to its corresponding hydroperoxo complex, $[(en)_2(NH_3)CoO_2HCo(en)_2(NH_3)]^{5+}$ (**2**). During this act, RSH and R′SH are quantitatively oxidized to their respective disulfides. Dissolved copper, even at the impurity level, dramatically catalyzes the reaction such that the direct reactions are inaccessible. Nevertheless, the catalyzed path can be masked completely with 0.20 mM dipicolinic acid and it can be determined that the direct reactions are first-order in [**1**], in [total thiol] and in basicity. Rate decreases linearly with increasing mol% of D_2O in the solvent. H-atom (H^+ + e) transfer from thiols to superoxide in **1** seems logical for the conversion of **1** to **2**.

$$\begin{tikzcd}
{[(en)_2(NH_3)CoO_2Co(en)_2(NH_3)]^{5+} + H^+} \arrow[r, shift left, "K"] \arrow[d, "k"', "RSH"] & {[(en)_2(NH_3)CoO_2Co(en)_2(NH_3)]^{6+}} \arrow[l, shift left] \\
{[(en)_2(NH_3)CoO_2HCo(en)_2(NH_3)]^{5+} + RS^\bullet} &
\end{tikzcd}$$

Contributory Paper-62

A graphene modified quinoxaline derivative based iron nanocomposite for optical sensing of Prostate Specific Antigen (PSA)

Shalmali Basu[a], Debashree Das[a], Zarina Ansari[a], Nabakumar Rana[b], David Morgan[c], Sanjay Dutta[d] and Kamalika Sen*[a]
[a]Department of Chemistry, [b]Department of Physics,
University of Calcutta,
92, Acharaya Prafulla Chandra Road,
Kolkata-700 009, India
[c]Cardiff Catalysis Institute, School of Chemistry, Cardiff University,
Park Place, Cardiff, CF10 3AT, U.K.
[d]Department of Organic and Medicinal Chemistry,
CSIR-Indian Institute of Chemical Biology,
4, Raja S. C. Mullick Road,
Kolkata-700 032, West Bengal, India
E-mail: kamalchem.roy@gmail.com
kschem@caluniv.ac.in

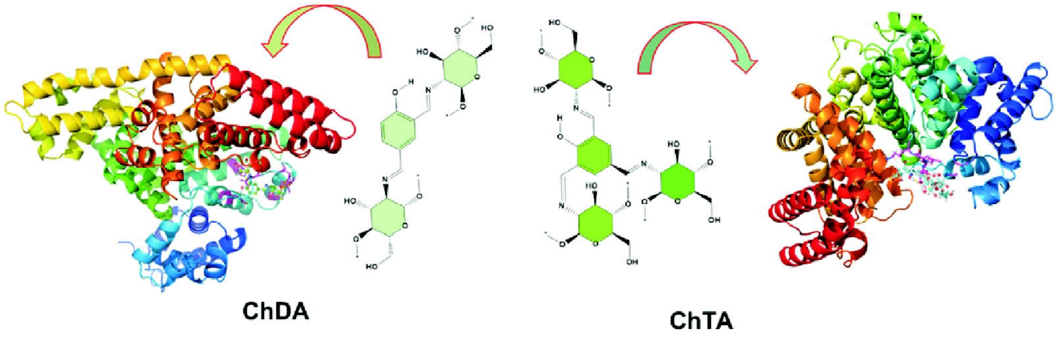
Herein we report an easy, rapid and cost-effective method for optical sensing of a prostate cancer biomarker prostate specific antigen (PSA) using a novel nanocomposite. The material is a synthetic quinoxaline derivative-based iron nanocomposite fabricated on graphene nanoplatelet surface (1d-Fe-Gr). Enhanced efficacy of synthesized 1d-Fe-Gr to sense PSA in serum medium with an impressive limit of detection (LOD) value of 0.879 pg/mL using UV-visible absorption spectroscopy is established here. Moreover, presence of interfering biomolecules like glucose, cholesterol, bilirubin and insulin in serum improves the detection threshold significantly. In presence of these biomolecules, which indicate physiological conditions for comorbidities like diabetes, hypercholesterolemia or hepatic disorders, etc., the LOD values improve significantly as compared to healthy conditions in the range 0.624–0.879 pg/mL. Thus, this proposed detection method could also be applied efficiently to the patients suffering from these pathophysiological disorders. These biomolecules can also be added externally to improve the sensing ability. Fluorescence, Raman and circular dichroism spectroscopy are used to study the underlying mechanism.

Contributory Paper-63

Establishment the flexibility improved the binding ability functionalized sugar based hydrogel

Shubhankar Ghorai
Indian Institute of Engineering Science and Technology, Shibpur,
Howrah, West Bengal
E-mail: shubhankar234@gmail.com

The modification at the branching of chitosan using 4-hydroxyisopthalaldehyde (ChDA) and 2-hydroxybenzene-1,3,5-tricarbaldehyde (ChTA) through chemically cross-linked has been structured for hydrogel fabrication. Both hydrogels produced mechanical properties, improved swelling capacity and delayed degradation for new cross linking-functionalized during experimental works. The swelling water ratio of this hydrogel makes it robust and elastic, providing a mechanical basis to keep the hydrogel strong and steady. A remarkable self-fluorescence behavior has been witnessed. The distinct photo-sensitiveness has been studied thoroughly as time, temperature and solvent-dependent spectral analysis to establish the ESIPT mechanism and improve stability in various conditions. Detailed instrumental-structural evaluations are explored as required and optimized the gel skeleton and photo activities are using DFT calculations. Hydrogel interaction with bovine serum albumin (BSA) was examined in both cases. To investigate how BSA interacts with hydrogels under physiological conditions, spectroscopic techniques such as fluorescence, UV absorption, and FT-IR were used. To study the interaction between hydrogels and BSA, we measured the quenching of intrinsic fluorescence of BSA at three different temperatures. We determined the binding constant (K), Stern-Volmer quenching constant (K_{SV}) and the number of binding sites.



Graphical Representation

Contributory Paper-64

Role of efficient charge transfer at the interface between mixed phase copper-cuprous oxide and conducting polymer nanostructures for green fuel generation

Susmita Bera[a], Sourabh Pal[a] and Srabanti Ghosh[a,b]
[a]Energy Materials & Devices Division,
CSIR - Central Glass and Ceramic Research Institute
Raja S. C. Mullick Road, Jadavpur, Kolkata-700 032
[2]Academy of Scientific & Innovative Research (AcSIR),
Ghaziabad, India
E-mail: sbera876@gmail.com

Photocatalytic water splitting is regarded as a sustainable technology capable of producing green hydrogen generation[1,2]. However, the present technology have been limited with high cost, low solar light absorption and charge separation efficiency which in turn influence the overall performance of photocatalyst. Fabrication of heterostructure as a promising strategy for efficient light absorption, charge transfer, prolonged lifetime of the charge carriers and boosts the photocatalytic redox reactions[3]. Herein, a novel, multiphase copper-cuprous oxide/ PPy heterostructures has been developed to understand the role of multiple oxidation states in water reduction and oxidation reaction. The presence of mixed phase shows higher catalytic activity with eight times greater H_2 generation rate compared to single phase. Interestingly, the copper-cuprous oxide/PPy heterostructures exhibited higher charge carrier density, low resistivity and five times greater photocurrent density compare to Cu_2O/PPy. A p-p-n junction may be formed between polymer and metal oxide interfaces which further improves the catalytic activity by creating an internal electric field. Notably, the separation and transfer of photoexcited charge carriers have been greatly improved between copper-cuprous oxide nanocubes and PPy nanofibers manifested by femtosecond transient absorption spectroscopy. Thus, present study highlights the role of mixed oxide and their heterostructure formation with conducting polymer for photocatalytic H_2 and O_2 generation.

References

1. S. Ghosh, N. A. Kouame, L. Ramos, S. Remita, A. Dazzi, A. Deniset-Besseau, P. Beaunier, F. Goubard, P.-H. Aubert and H. Remita, Nanostructured conducting polymers for energy applications: towards a sustainable platform. *Nat. Mater.*, 2015, **14**, 505-511.
2. S. Ghosh, M. Thandavarayan and R. N. Basu, Nanostructured conducting polymers for energy applications: towards a sustainable platform. *Nanoscale,* 2016, **8**, 6921-6947.
3. S. Ghosh, D. Rashmi, S. Bera and R. N. Basu, Functionalized conjugated polymer with plasmonic Au nanoalloy for photocatalytic hydrogen generation under visible-NIR. *Int. J. Hydrogen Energy,* 2019, **44**, 13262-13272.

Contributory Paper-65

Evaluation of pesticidal residue in the soil of maihar region of satna, M. P., India

Asha Kalwani and Neelam Richhariya
Department of Chemistry,
Girls P.G. College,Satna,
APSU, Rewa, Madhya Pradesh, India
E-mail: ashakalwani33@gmail.com

In the present study, Maihar region of Satna has been selected for evaluation of pesticidal residue present in the soil. Selected soil samples taken from specific sites and analysed on the basis of 76 different types of pesticides used in this area. It was found that only concentration of pendimethalin was above detectable limit and the places where concentration of pendimethalin was high and exhibited adverse effect not only human but also on all biological systems. People of these places are slightly affected by pendimethalin concentration but not at a hazardous level.

Contributory Paper-66

Visible-light driven enhanced photocatalytic water splitting activity of ZnO nanocrystals by simultaneously metal doping and coupling with polypyrrole nanofibers

Sourabh Pal[a], Aritra Banerjee[a] and Srabanti Ghosh[a,b]
[a]Energy Materials & Devices Division,
CSIR - Central Glass and Ceramic Research Institute
Raja S. C. Mullick Road, Jadavpur, Kolkata-700 032
[b]Academy of Scientific & Innovative Research (AcSIR),
Ghaziabad, India
E-mail: sourabh96pal@gmail.com

Solar-to-hydrogen (H_2) conversion has been regarded as a sustainable and renewable technique to address aggravated environmental pollution and global energy crisis. Solar fuels technologies are analogous to natural photosynthesis and the use of solar energy to convert water into fuels are sustainable and produce no net emissions of carbon dioxide[1,2]. The most critical aspect in this technology is to develop highly efficient and stable photocatalysts, especially noble metal-free photocatalysts[3]. In this work, ZnO nanoparticles modified with metal doping as well as functionalized with polypyrrole (PPy) nanofibers have been used as photocatalysts for water splitting. A shift in absorption in visible region have been observed for ZnO after modification with PPy nanofibers. The significant lowering of band gap obtained for Bi-ZnO/PPy (~1.25 eV) compared to pure ZnO, (~3.2 eV) and polypyrrole (~1.86 eV). The Bi doped ZnO/PPy nanohybrid showed a H_2 generation of 13.5 mmol/h, ~ 2.4 time higher than pure PPy nanofibers (5.7 mmol/h). The as formed nanohybrids have manifested efficient charge separation as observed in impedance spectra. Present study identifies a novel approach towards highly efficient photocatalysts for water splitting and green H_2 generation.

References

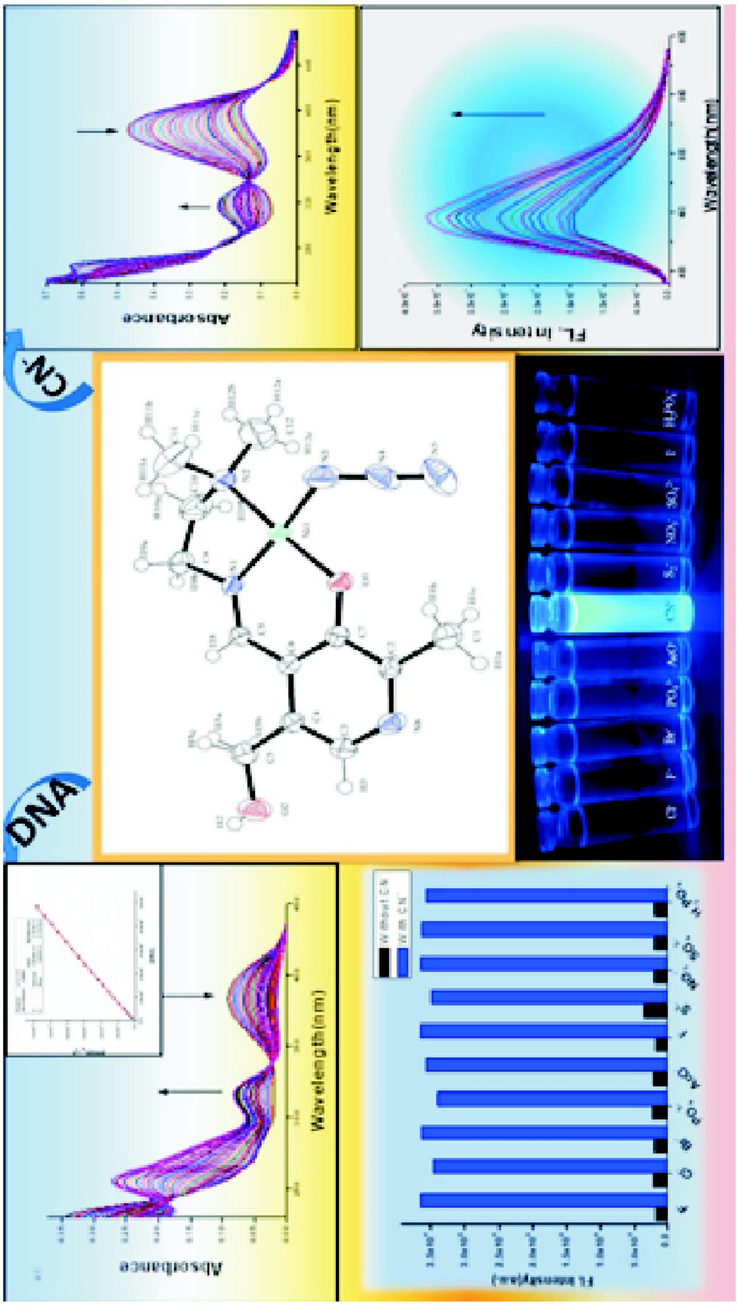
1. S. Ghosh, N. A. Kouame, L. Ramos, S. Remita, A. Dazzi, A. Deniset-Besseau, P. Beaunier, F. Goubard, P.-H. Aubert and H. Remita, Nanostructured conducting polymers for energy applications: towards a sustainable platform. *Nat. Mater.*, 2015, **14**, 505-511.
2. S. Ghosh, H. Remita and R. N. Basu, Significantly enhanced photocatalytic reduction of Cr(VI) on ZnO-conducting polymeric nanofibers heterojunction under visible-light irradiation. *Appl. Catal B.*, 2018, **239**, 362-372.
3. S. Sardar, P. Kar, H. Remita, B. Liu, P. Lemmens, S. K. Pal and S. Ghosh, Enhanced charge separation and FRET at heterojunctions between semiconductor nanoparticles and conducting polymer nanofibers for efficient solar light harvesting. *Sci. Rep.*, 2015, **5**, 1-14.

Contributory Paper-67

Selective turn on fluorescence sensing of cyanide using pyridoxal platform of a Ni(II) complex

Antu Mondal and Shyamal Kumar Chattopadhyay*
Department of Chemistry,
IIEST, Shibpur,
Howrah, West Bengal
E-mail: antumondal0102@gmail.com

Cyanide is a very toxic pollutant for aquatic life and environment. Analytical methods of quantitative assay of cyanide, which are rapid, sensitive (low limit of detection) and cost effective, are in great demand. Colorimetric and fluorimetric methods are ideally suited for this purpose. In this report we describe a Ni(II) complex containing a pyrdoxal platform for rapid and sensitive fluorimetric estimation of cyanide. The square planar Ni(II) complex, $[Ni(L)(N_3)]\cdot 3H_2O$, where the ligand LH = 4-[(2-dimethylamino-ethylimino)-methyl]-5-hydroxymtheyl-2-methyl-pyridin-3-ol, a Schiff base formed between pyridoxal and (2-dimethylamino)ethyl amine, has been synthesized and characterized by various spectroscopic techniques as well as by single crystal X-ray structure determination. The complex was found to selectively bind CN^- in presence of other biologically important anions like F^-, Cl^-, Br^-, I^- and OAc^-, S^{2-}, NO_3^-, PO_4^{3-}, SO_4^{2-}, $H_2PO_4^-$ in tris-HCl/NaCl buffer [pH = 7.4]) and it can be monitored by fluorescence turn on or by UV-Visible spectroscopy. The binding constant of the complex with CN^- was estimated as 2.046×10^{14} M^{-2} and the limit of detection (LOD) was 9 nM, the LOD being considerably lower than the maximum permissible level of cyanide ions (1.9 μM) in drinking water recognized by the WHO. The effects of pH and temperature on the sensing are also investigated. The Ni(II) complex is also found to bind calf-thymus DNA very strongly and the apparent binding constant (K_{app}) was determined as 1.33×10^7 M^{-1} by fluorescence quenching of ethidium bromide-DNA adduct by the complex.



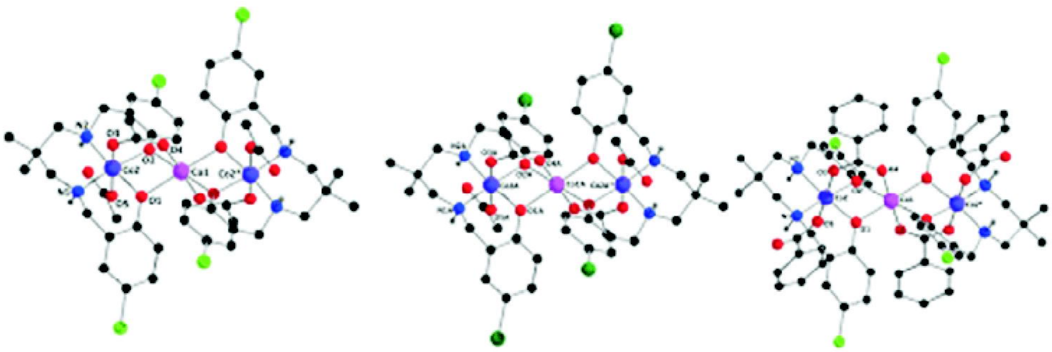
Contributory Paper-67

Contributory Paper-68

Synthesis and characterization of a series of carboxylate bridged trinuclear mixed valence cobalt complexes

Sudip Bhunia and Shouvik Chattopadhyay*
Department of Chemistry, Inorganic Section,
Jadavpur University,
Kolkata-700 032, India
E-mail: sudipchem1295@gmail.com

Three linear mixed-valence trinuclear cobalt(III)-cobalt(II)-cobalt(III) complexes, $[Co^{II}\{(\mu\text{-}L^1)(\mu\text{-}OOCCH_3)Co^{III}(OOCCH_3)\}_2]\cdot 4H_2O$ **(1)**, $[Co^{II}\{(\mu\text{-}L^2)(\mu\text{-}OOCCH_3)Co^{III}(OOCCH_3)\}_2]\cdot 4H_2O$ **(2)** and $[Co^{II}\{(\mu\text{-}L^1)(\mu\text{-}OOCPh)Co^{III}(OOCPh)\}_2]$ **(3)**, have been synthesized using two tetradentate N_2O_2 donor 'reduced Schiff base' ligands, H_2L^1 (2,2-dimethyl-1,3-propanediyl)bis(iminomethylene)bis(4-chlorophenol) and H_2L^2 (2,2-dimethyl-1,3-propanediyl)bis(iminomethylene)bis(4-bromophenol), and acetate or bezoate as anionic co-ligands. The complexes have been characterized by single crystal X-ray diffraction study and different spectral analyses.



Contributory Paper-69

Stabilization of CO_2 as zwitterionic carbamate within a Coordination Polymer (CP): Synthesis, structure and anions sensing behaviour of Tb-CP composite

Sourav Sarkar and Partha Mahata
Department of Chemistry,
Jadavpur University,
Kolkata-700 032, India
E-mail: souravsarkarchem@gmail.com

A new gadolinium (III) based coordination polymer (CP), [Gd(3,5-pydc)$_{1.5}$(CO_2)$_{0.5}$(H_2O)$_4$].3H_2O (where 3,5-pydc = 3,5-pyridinedicarboxylate), **1**, has been successfully synthesized using slow diffusion method at room temperature. Single crystal X-ray diffraction study of **1** confirmed one dimensional ladder like structure. The Gd^{3+} ions are in distorted tricapped trigonal prismatic geometry. Two types of 3,5-pydc ligands are present in the structures – in one case the pyridine nitrogen remain vacant whereas in other case the pyridine nitrogen coordinated with CO_2 to form zwitterionic carbamate. The phase purity of **1** has been confirmed by powder X-ray diffraction, thermogravimetric analysis and IR spectroscopic studies. Aqueous dispersion of compound **1** gives weak luminescence emission at 385 nm upon excitation at 270 nm. To explore ligand sensitized metal centre luminescence, we have prepared a composite by mixing the CP with Tb^{3+} ions (**Tb@1**). The formation of the composite has been confirmed by the IR spectroscopic studies in solid state. The composite showed excellent ligand sensitized metal centre luminescence. We have utilized this luminescence property for the sensing of anions in aqueous medium. The composite shows luminescence quenching behaviour in presence of $Cr_2O_7^{2-}$, CrO_4^{2-}, NO_2^{-} with high sensitivity. The limits of detections are 147 ppb, 142 ppb and 20 ppb, respectively. The selectivity experiments show that the detection of these three anions is highly selective in presence of other common anions. Details experimental studies suggest that the preferable interaction of the three anions with the Tb^{3+} ions inside the composite and the reduction of the excitation energy, probably, responsible for the quenching behaviour.

Contributory Paper-70

A new porous Cd based MOF and its multifunctional properties

Priyanka Manna and Partha Mahata*
Department of Chemistry,
Jadavpur University,
Kolkata-700 032, India
E-mail: priyanka.moni.chem@gmail.com

A Cd(II)-based metal–organic framework (MOF) [Cd(TPIM)(PDA)] (PDA = 1,4-phenylenediacetic acid and TPIM = 4,5-tri-4-pyridyl-1H-imidazole) has been synthesized by hydrothermal method and characterized by single-crystal X-ray analysis, powder X-ray diffraction, Fourier Transform Infrared (FTIR) and thermogravimetric analysis (TGA). The single crystal X-ray studies show two-dimensional structure. The Cd-MOF showed trifunctional properties: (i) selective and great efficient adsorbent of organic dyes namely RBBR and OG, (ii) luminescence sensor toward Fe^{3+}, Cr^{3+} and Al^{3+} ions *via* luminescence quenching effect with good sensitivity and selectivity and detection limit equivalent to 75, 257 and 107 ppb of Fe^{3+}, Cr^{3+}, Al^{3+} metal ions respectively, (iii) comparable gas adsorption capacity towards CO_2, N_2 and H_2. In particular, the MOF exhibits excellent selectivity toward anionic Remazol Brilliant Blue R (RBBR) and Orange G (OG) dye adsorption and separation. It also displays intense luminescence along with quenching effect in the presence of trace amount of Fe^{3+}, Cr^{3+} and Al^{3+} ions making it a potential probe for detecting these metal ions. In addition, the Cd-MOF has also exhibited 64.5 cm^3/g of CO_2 uptakes at 1 bar. The synthesis, structure and properties of the Cd-MOF will be described and discussed in details.

Contributory Paper-71

Effect of hydrogen bonding on the luminescence lifetime: A case study based on two new related Cd-based coordination polymers

Akash Kumar Chandra, Priyanka Manna and Partha Mahata*
Department of Chemistry,
Jadavpur University, Jadavpur,
Kolkata-700 032, India
E-mail: parthachem@gmail.com

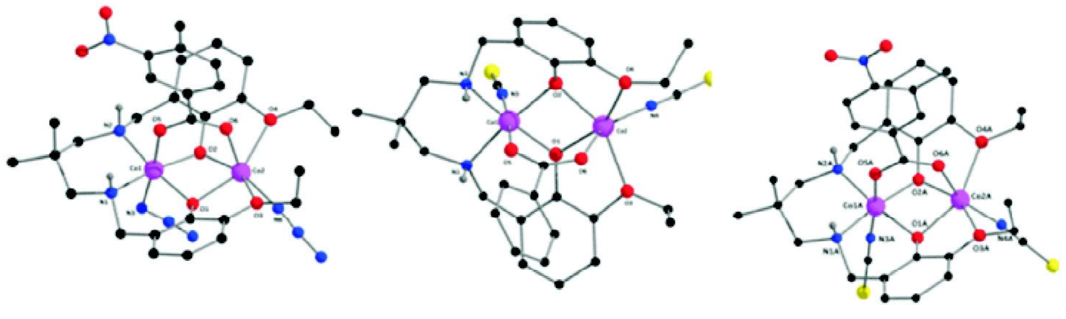
Two new coordination polymers of formulas $[Cd_2(2,3\text{-pzdc})(tz)_2]$ (**1**) and $[Cd_2(2,3\text{-pzdc})(dtz)_2]$ (**2**) {2,3-pzdc = 2,3-pyrazine dicarboxylate, tz = 1,2,4-triazolate, dtz = 3,5-diamino-1,2,4-triazolate)} were synthesized *via* hydrothermal techniques. Both the compounds were characterized by single-crystal X-ray analysis, powder X-ray diffraction, Fourier Transform Infrared (FTIR) and thermogravimetric analysis (TGA). Single crystal X-ray analysis shows both the structures are three-dimensional in nature and connectivity wise they are similar with each other. In compound **2**, the presence of N-H…O hydrogen bond interactions further stabilized the structure. Aqueous dispersion of both the compounds show strong duel emission - one emission around 353 nm and another one is at 369 nm upon excitation at 280 nm. Lifetime studies from time resolved spectra show 0.82 and 0.60 ns for compound **1** and 2.02 and 1.78 ns for compound **2**. The higher lifetime of excited states in case of compound **2** establish the role of hydrogen bond interactions to reduce the non-radiative decay processes.

Contributory Paper-72

Synthesis and characterization of a series of dinuclear mixed valence cobalt(III), cobalt(II) complexes with a compartmental 'reduced Schiff base' ligand

Rabi Sankar Sarkar and Shouvik Chattopadhyay*
Department of Chemistry, Inorganic Section,
Jadavpur University,
Kolkata-700 032, India
E-mail: rssarkariitm@gmail.com

A series of mixed valance cobalt(III/II) complexes $[(N_3)Co^{III}L(\mu\text{-}O_2CR^1)Co^{II}(N_3)]$ (**1**), $[(SCN)Co^{III}L(\mu\text{-}O_2CR^2)Co^{II}(NCS)]$ (**2**) and $[(SCN)Co^{III}L(\mu\text{-}O_2CR^3)Co^{II}(NCS)]$ (**3**) {R^1CO_2H = 4-methyl-3-nitrobenzoic acid; R^2CO_2H = benzoic acid; R^3CO_2H = 3-methyl-4-nitrobenzoic acid} have been synthesized and characterized. Each complex has been structurally characterized by single crystal X-ray diffraction and spectral analysis. Both the cobalt centers in these dinuclear complexes adopt distorted-octahedral geometry, where the cobalt(III) center resides at the inner N_2O_2 cavity and the cobalt(II) center resides at the outer O_4 cavity of the reduced Schiff base.

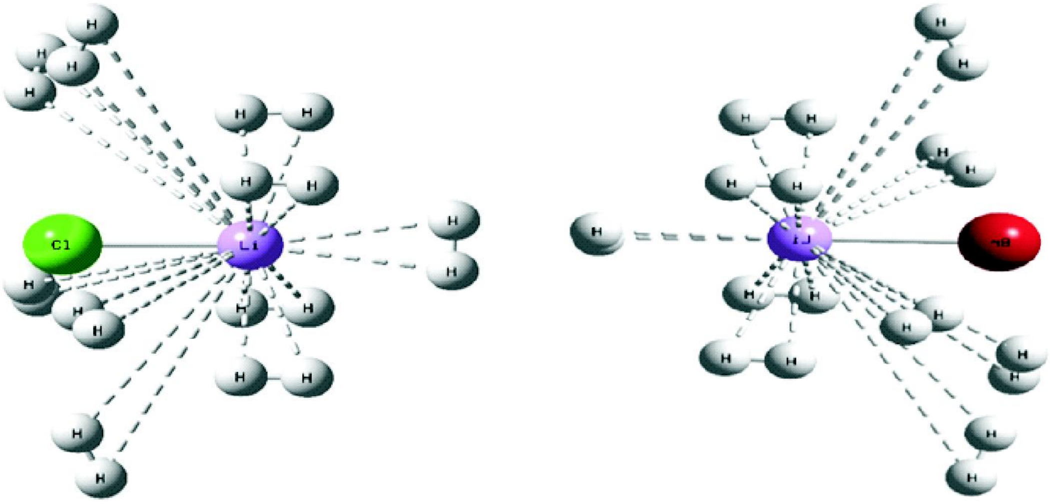


Contributory Paper-73

Hydrogen storage on LiCl/Br surface at low temperature

Anjana Ghosh[a,b] and Gourisankar Roymahapatra[a]
[a]School of Applied Science and Humanities,
Haldia Institute of Technology,
Haldia-721 657, India
[b]A. B. Polypacks Pvt. Ltd.,
Howrah-711 409, India
E-mail: anjanaghosh04@gmail.com

Lithium Chloride (LiCl) and lithium bromide (LiBr) found as promising template for hydrogen storage at low temperature been expressed in this article. The structure, chemical reactivity of the derived templates has been studied based on density functional theory (DFT). The adsorption process is found to quasisorption in nature. The molecular hydrogen interacts with building blocks (with Li^+ centre) through electrovalent interaction and a single LiCl/LiBr molecule is capable of absorbing 10 H_2 with a high gravimetric wt% value (32.00 for LiCl and 18.71 for LiBr) which are found to be promising systems as per standard. The Gibbs free energy changes suggest a spontaneous hydrogen adsorption process at cryogenic temperature.



LiCl@10H_2 **LiBr@10H_2**

References

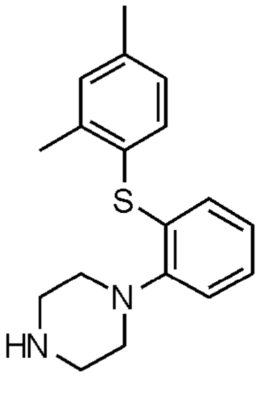
1. *ES Energy & Environment*, 2022. https://dx.doi.org/10.30919/esee8c756.
2. *Engineered Science,* 2022, **18**, 98-104. https://dx.doi.org/10.30919/es8d658.

Contributory Paper-74

Design, synthesis and biological evaluation of vortioxetine derivatives as new COX-1/COX2 inhibitors in human monocytes

Raju D. Chaudhari and Goutam Biswas*
Department of Chemistry,
Vivekananda Street, Cooch Behar,
Cooch Behar-736 101, West Bengal, India
E-mail: goutam@cbpbu.ac.in

In order to identify a suitable alternative for non-steroidal anti-inflammatory drugs (NSAIDs) we aimed to develop derivatives of vortioxetine, a multimodal anti-depressive drug, endowed of antioxidative as well as anti-inûammatory activity, leading to immunomodulatory effects on human monocytes/macrophages. It was reported that commonly used NSAIDs have many side effects, but most common is an increased risk of gastrointestinal ulcers and bleeds, heart attack and kidney disease. Even though there are some potent NSAIDs (like ibuprofen, naproxen, fenoprofen, diclofenac etc) are available in the market, literature is abundant with its gastric and other side effects because of the presence of free carboxylic group.The parent molecule vortioxetine (**1**) was synthesized in good yield and the different alkyl, aryl, sulfonyl, Urea derivatives were prepared based on their structural diversity and easy availability. These prodrugs seem to reduce the side effect but only very few research groups are now focused on developing carboxylic acid devoid NSAIDs. We developed a new set of heterocyclic compounds which will be devoid of any carboxylic acids. The newly synthesized compounds will be tested on human monocytes isolated from healthy donors, as inhibitors of superoxide



Vortioxetine

anion production, for cytokine gene expression, and for COX-1/2 gene expression and activity. Moreover, a docking study was performed to investigate enzyme–ligand interactions. Correlating experimental biological data to the molecular modelling studies, it emerged that among the novel compounds, shows good antioxidant and anti-COX-1 activities, good anti-COX-1/2 inhibitor and some of compounds was more specific versus COX-2.

References

1. Maria Talmon et al., *Bioorg. Med. Chem.*, 2020.
2. S. K. Suthar and M. Sharma, Recent developments in chimeric NSAIDs as safer anti-inflammatory agents, *Med. Res. Rev.*, 2015, **35**, 341-407.
3. M. Talmon, S. Rossi, A. Pastore, C. I. Cattaneo, S. Brunelleschi and L. G. Fresu. Vortioxetine exerts anti-inflammatory and immunomodulatory effects on human monocytes/macrophages. *Br. J. Pharmacol.*, 2018, **175**, 113-124.

Contributory Paper-75

A hydrothermal route for constructing lanthanum orthoferrite/reduced graphene oxide nanocomposite towards photocatalytic H_2 generation

Soumita Samajdar[a,b], Maitrayee Biswas[a], Susmita Bera[a], Srabanti Ghosh[a,b]
[a]Energy Materials & Devices Division,
CSIR - Central Glass and Ceramic Research Institute,
Raja S. C. Mullick Road, Jadavpur, Kolkata-700 032
[b]Academy of Scientific & Innovative Research (AcSIR),
Ghaziabad, India
E-mail: soumita.samajdar@gmail.com

Green hydrogen production via visible-light driven photocatalytic water splitting has received global attention, as it promotes the direct conversion of solar energy to chemical energy. Lanthanum orthoferrite ($LaFeO_3$) nanorods has been selected as photocatalysts due to its narrow band gap, ferroelectric behavior, high stability, non-toxicity and cost-effectiveness[1,2]. However, it is limited with fast charge carrier recombination rate. In order to overcome this limitation, $LaFeO_3$ has been combined with reduced graphene oxide (rGO) which exhibits superior electron mobility, high conductivity and large surface area. As an efficient, cost-effective and visible-light active photocatalyst, lanthanum orthoferrite/reduced graphene oxide nanocomposite has been synthesized via facile hydrothermal method. The as-prepared nanocomposites have been characterized by X-ray diffraction, Raman spectroscopy, transmission electron microscopy, X-ray photoelectron spectroscopy, and ultraviolet-visible diffuse reflectance spectroscopy. The photoelectrochemical properties of $LaFeO_3$/rGO nanocomposite have been studied in details to explore the charge transfer mechanism. The photocurrent density of the nanocomposite is 21 times higher than pure $LaFeO_3$. The $LaFeO_3$/rGO nanocomposite has been successfully used as photocatalyst for H_2 generation through water reduction under visible light. A significant enhancement in H_2 generation has been recorded for $LaFeO_3$/rGO nanocomposite(~ 112mM g^{-1} h^{-1}) as compared to pure $LaFeO_3$ (~ 14 mM g^{-1} h^{-1}).

References

1. C. Orak and A. Yüksel, Graphene-supported $LaFeO_3$ for photocatalytic hydrogen energy production. *Int. J. Energy Res.*, 2021, **45**, 12898-12914.
2. R. D. Kumar, R. Thangappan and R. Jayavel , Facile preparation of $LaFeO_3$/rGO nanocomposites with enhanced visible light photocatalytic activity. *J. Inorg. Organomet. Polym.*, 2017, **27**, 892-900.

Contributory Paper-76

Synthesis of xanthopyran and ring-enlarged siblings

Shyamasankar Mandal, Shyamal Das and Shital K. Chattopadhyay
Department of Chemistry,
University of Kalyani,
Kalyani-741 235, West Bengal, India
E-mail: shyamasankarmandal@gmail.com

We[1] and others[2], have recently reported synthesis and cellular evaluation of the anti-cancer drug acrinomycin (**1**, Gig. 1) and some of its ring-enlarged analogues. The corresponding oxa-analogue II has also been studied. However, the ring-enlarged analogues IV and V are yet to be evaluated. In continuation of our ongoing programme[3] on the synthesis of biologically relevant benzoxepins and benzoxocins, we have developed a synthetic route to the ring-enlarged derivatives IV and V starting from the known dihydroxy xanthone derivative II.

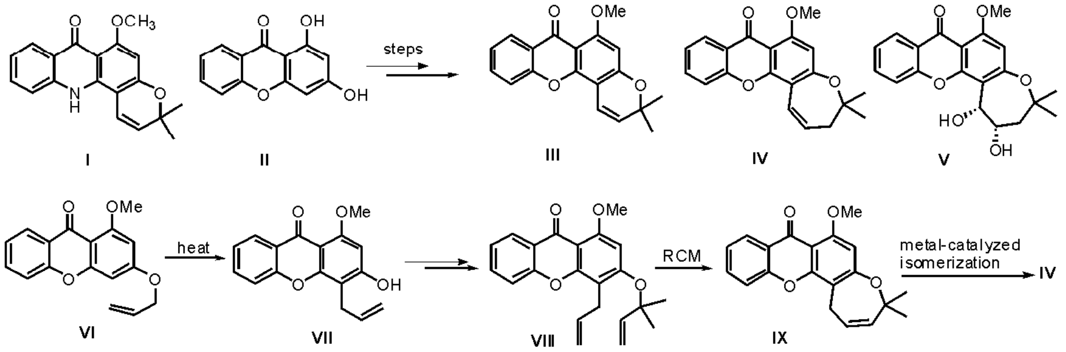


Fig. 1. Biologically relevant xanthone derivatives as analogues of acronycine.

Thus, starting from II, sequential allylation and methylation produced the corresponding ether VI. This on Claisen rearrangement of VI to VII followed by further allylation of the latter produced the new allyl ether VIII. Ring-closing metathesis with Grubbs 1st generation catalyst led to the smooth formation of the oxepin derivative ix. OsO_4-mediated dihydroxylation of IX led to the diol V. The cellular evaluation of the newly prepared compounds was conducted. The results obtained will be presented.

References

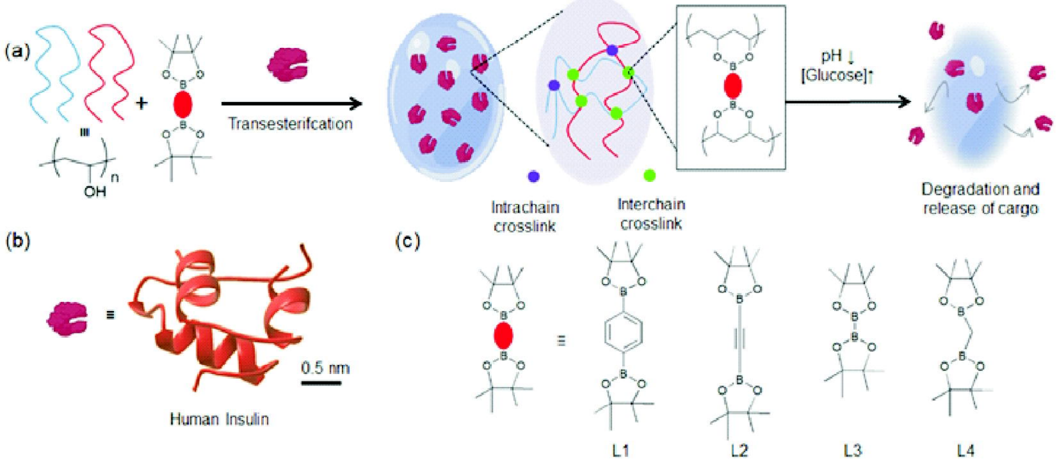
1. J. Banerjee, I. Kundu, S. Zhang, S. Wen and S. K. Chattopadhyay, *ACS Omega,* 2019, **4**, 6106-6113.
2. T. Mandal, S. Karmakar, A. Kapat and J. Dash, *ACS Omega*, 2021, **6**, 27062-27069.
3. S. K. Chattopadhyay, S. Maity, B. Pal and S. Panja, *Tetrahedron Lett.,* 2002, **43**, 5079.

Contributory Paper-77

Repurposing pinacol esters of boronic acids for tuning viscoelastic properties of glucose-responsive polymer hydrogels: Effects on insulin release kinetics

A. Ali[a], S. Nouseen[a], S. Saroj[b], M. Shegane[c], P. Majumder[a],
Aarti Puri[a], T. Rakshit[b], D. Manna[c] and S. Pal*[a]
[a]Department of Chemistry,
Indian Institute of Technology, Bhilai,
Raipur-492 015, Chhattisgarh, India
[b]Department of Chemistry,
Shiv Nadar University,
Greater Noida-201 314, Uttar Pradesh, India
[c]Department of Chemistry,
Indian Institute of Science Education and Research,
Bhopal-462 066, Madhya Pradesh, India
E-mail: suchetanp@iitbhilai.ac.in

In the era of the diabetes pandemic, Injectable hydrogels (HGs) capable of releasing the desired amount of insulin under hyperglycemic conditions will significantly advance smart insulin development. Several smart boronic acid-based polymer HGs release insulin under high-glucose conditions. However, the correlation of insulin release characteristics with rheological properties is not well understood yet. Herein, we report a generalized and facile fabrication strategy of a new class of glucose-responsive hydrogels by crosslinking a biocompatible polymer, poly(vinyl alcohol) with pinacol ester of bisboronic acids via transesterification reactions. We show the versatility of the method by fabricating four hydrogels with diverse rheological properties. The HGs embody more than 70% water amenable for hosting insulin in the matrix. HG with high storage modulus, derived from 1,4-Benzenediboronic acid bis(pinacol) ester releases ~3 fold less insulin compared to softer HGs derived from Acetylene-1,2-diyl bis(boronic acid pinacol ester) and Bis[(pinacolato)boryl]methane under hyperglycemic conditions. We find that HG derived from Bis[(pinacolato)boryl]methane crosslinker exhibits superior insulin release properties due to the softness of the hydrogel matrix. We further show that the newly formulated gel is injectable without any structural change in the released insulin molecules and does not cause cytotoxicity. We believe that glucose-responsive hydrogels with tunable viscoelastic properties will pave the way for developing a variety of hydrogels with programmable insulin release properties.



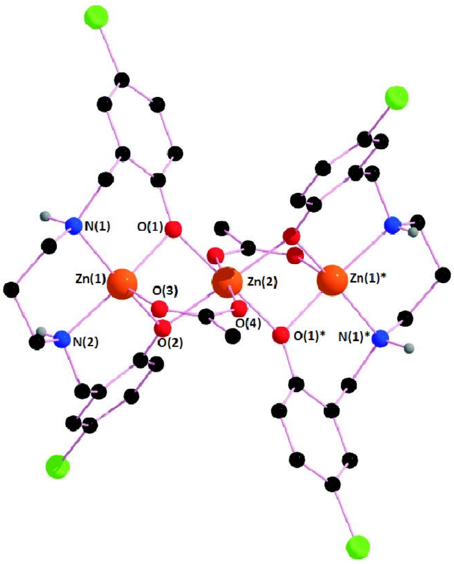
Schematic representation of the glucose-responsive hydrogels developed in this study. PVA chains are crosslinked with pinacol esters of bisboronic acid via a thermodynamically favorable transesterification reaction and entrap molecular guests. There are two different crosslinks: interchain (green) and intrachain (purple). These HGs are expected to undergo structural degradation under low pH and high glucose environments releasing (b) The three-dimensional structure of insulin (PDB: 3I40). (c) Chemical structures of four pinacol ester of bisboronic acid used in this study: L1: 1,4-Benzenediboronic acid bis(pinacol) ester, L2: 1,2-diyl bis(boronic acid pinacol ester), L3: Bis(pinacolato) diboron, L4: Bis(pinacolato) borylmethane.

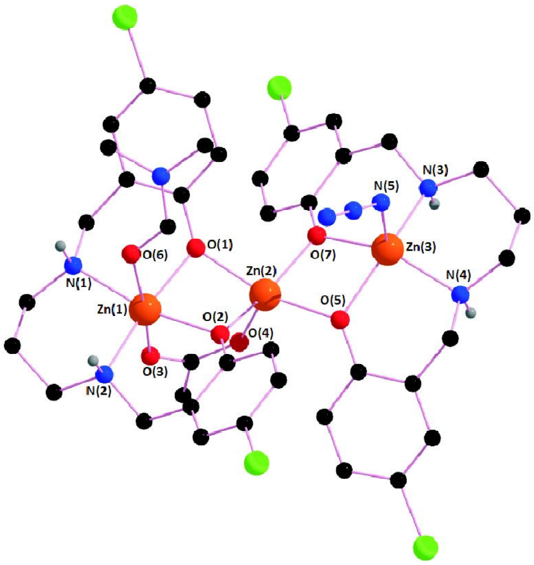
Contributory Paper-78

Synthesis and characterization of trinuclear zinc complexes with the reduced analogue of an N_2O_2 donor salen type Schiff base ligand

Puspendu Middya and Shouvik Chattopadhyay*
Department of Chemistry, Inorganic Section,
Jadavpur University,
Kolkata-700 032, India
E-mail: puspendumiddya@gmail.com

Two zinc complexes $[\{(\mu\text{-}CH_3COO)ZnL\}_2Zn]\cdot 2DMF$ (**1**) and $[\{(DMF)LZn(\mu\text{-}CH_3COO)LZn_2(N_3)\}]\cdot DMSO$ (**2**) $\{H_2L$ = (1,3-propanediyl)bis(iminomethylene)bis(5-chlorophenol)$\}$ have been synthesised and characterized by spectral analysis and single crystal X-ray diffraction. The complexes have been used to sense nitroaromatic explosives by turn off fluorescence response.



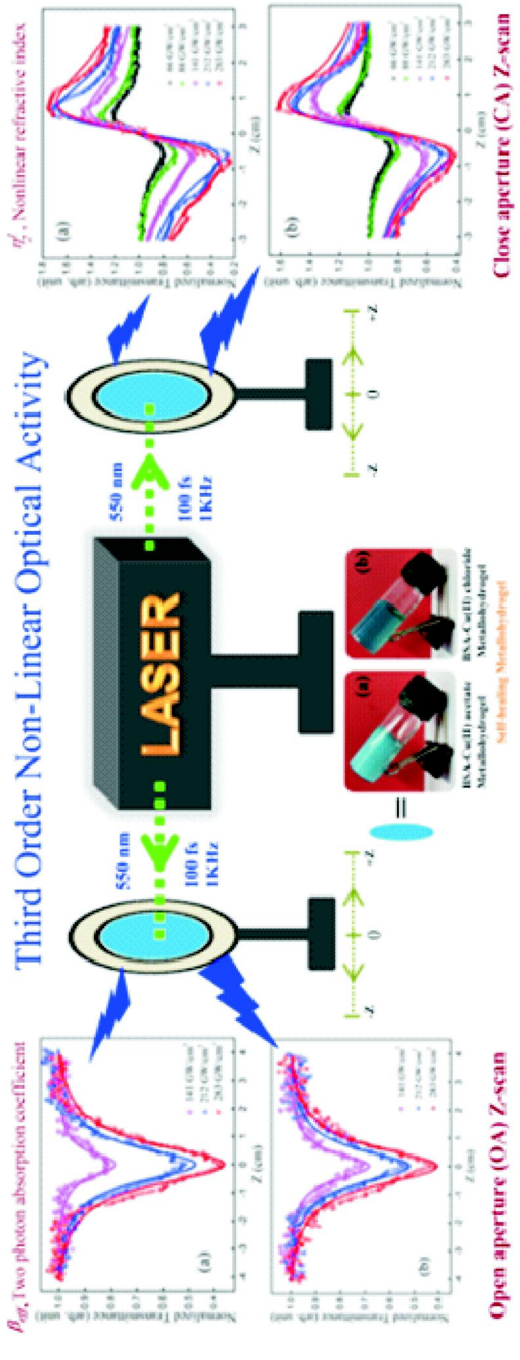


Contributory Paper-79

Protein based self-healing Cu(II)-metallohydrogels: Efficient third order non-linear optical materials

Santanu Majumdar* and Biswajit Dey
Department of Chemistry,
Visva-Bharati University,
Santiniketan-731 235, India
E-mail: santanumajumdar049@gmail.com

Protein based two self-healing Cu(II)-metallohydrogels named as BSA-CuA and BSA-CuCl have been synthesized by the mixing acetate and chloride salts of Cu(II) distinctly with the protein Bovinae Serum Albumin (BSA) in water medium. Experimentally investigated rheological parameters of both synthesized metallohydrogels not only expose the viscoelastic semi-solid nature and mechanical toughness but also reveal the self-healing properties of both metallohydrogel-materials. These two metallohydrogels exhibit excellent shape-sustaining, load-bearing and self-healing properties. Counter anions directed morphological variations of these metallohydrogels are visualized through field emission scanning electron microscopic images. The structural compactness with a hierarchically stacked layer-type morphology has been found for the BSA based metallohydrogel with Cu(II) acetate salt (BSA-CuA), whereas, the block shaped agglomerated micro-structural assembly has been observed in BSA-CuCl gel with chloride anion. EDX elemental analyses of both the metallohydrogels confirm the presence of individual gel-forming constituents. The third order optical nonlinear susceptibility, $x^{(3)}$ of these synthesized metallohydrogels has been studied by Z-scan technique at wavelength 550 nm under femtosecond regime in the excitation intensity ranges from 66GW/cm^2 to 283GW/cm^2. Both metallohydrogels exhibit high value of positive nonlinear refractive index, n_2^1 and two photon absorption coefficient, β_{eff} which are very important for all-optical switching, optical limiting, and other photonic applications. The polarity possibly associated to self-healing property of these two synthesized metallohydrogels has been justified through the experimentally measured high value of optical non-linearity. Out of the two metallohydrogel samples studied, BSA-CuA with the organic type acetate counter anion shows better nonlinear refraction as well as nonlinear absorption as compared to BSA-CuCl having inorganic type chloride counter anion in the Cu(II)-salt used for the individual metallohydrogel preparation. Both the metallohydrogels can be used in a number of fields like integrated optics, optical switching devices, optical signal processing, and optical limiting for future applications.



Reference

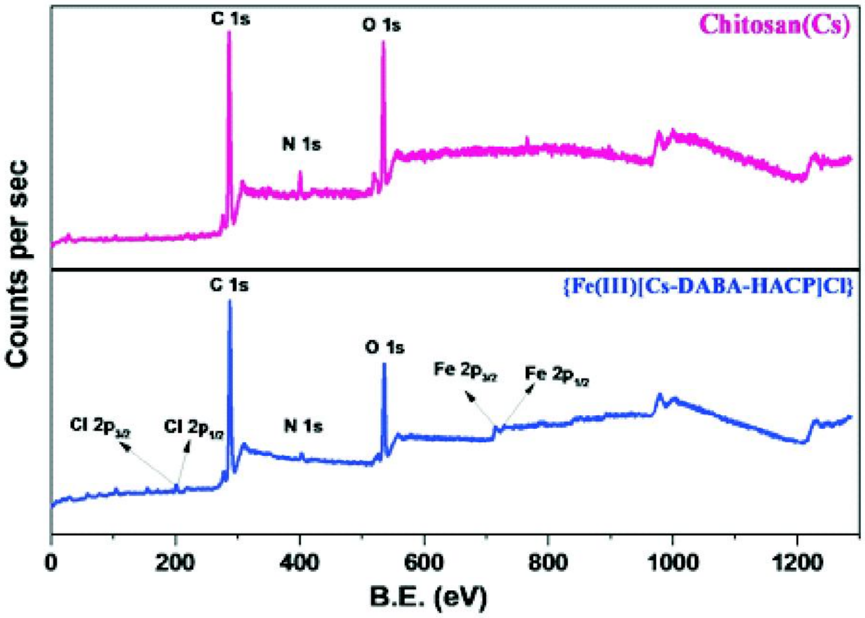
ACS, *Appl. Electron. Mater.*, 2020, **2**, 3678-3685.

Contributory Paper-80

The catalytic performance of chitosan based Fe(III) catalyst {Fe(III)[Cs-DABA-HACP]Cl}

Neha Tiwari and Savita Khare*
School of Chemical Sciences,
Devi Ahilya University,
Takshashila Campus, Khandwa Road,
Indore-452 001, Madhya Pradesh, India
E-mail: tneha3902@gmail.com
kharesavita@rediffmail.com

We have developed a new heterogeneous catalyst, chitosan based Fe(III) catalyst, {Fe(III)[Cs-DABA-HACP]Cl} by treating Fe(III) Schiff base metal complex with chitosan. The newly prepared heterogeneous catalyst, {Fe(III)[Cs-DABA-HACP]Cl} was analyzed by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray analysis (EDX), Fourier transform infrared spectroscopy (FTIR), Thermo gravimetric analysis (TGA), X-ray powder diffraction (XRD) etc.



The catalytic performance of prepared heterogeneous Fe(III) catalyst was tested for the cyclopentene oxidation using 70% *tert*-butylhydroperoxide (TBHP) as an oxidant. The cyclopentene oxidized to cyclopentenone. The 52.09% conversion of cyclopentene with 100% selectivity for cyclopentenone was obtained after 2 hours of reaction. The catalyst was recyclable upto 7 cycles under optimized conditions. The prepared catalyst was highly recoverable and easy to handle, easy to separate.

Contributory Paper-81

Oxidative decarbethoxylation reactions of benzylic C(sp^3)-H of ethyl arylacetates

Anjali Jaiswal and Krishna Nand Singh
Department of Chemistry,
Institute of Science,
Banaras Hindu University,
Varanasi- 221 005, India
E-mail: anjalijaiswal354979@gmail.com

The ethyl arylacetes is commercially available material in which the electrophilic as well as nucleophilic centre is generated by the activation of benzylic C(sp^3)-H to construct the C-C/C-heteroatom bond by oxidative deesterification[1]. 3-Acylated indoles are especially important as they constitute the core nucleus of many alkaloids, inhibitors of HIV-1 integrase, anticancer compounds and antidiabetics[2].

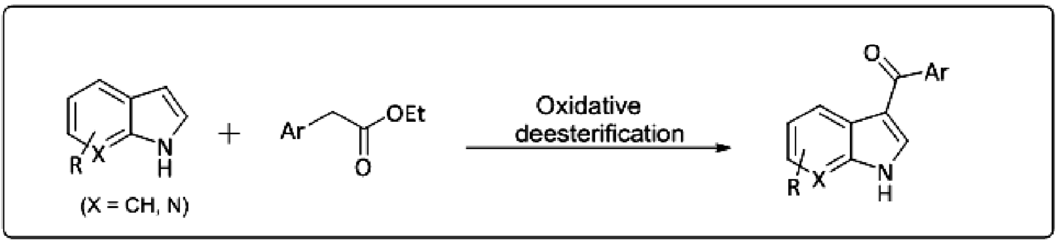


Fig. 1. Synthesis of 3-acylindoles.

References

1. C. L. Sun and Z. J. Shi, *Chem. Rev.*, 2014, **114**, 9219.
2. (a) T. Vasiljevik, L. N. Franks, B. M. Ford, J. T. Douglas, P. L. Prather, W. E. Fantegrossi and T. E. Prisinzano, *J. Med. Chem.,* 2013, **56**, 4537;

   (b) M. L. Barreca, S. Ferro, A. Rao, L. D. Luca, M. Zappala; A.-M. Monforte, Z. Debyser, M. Witvrouw and A. Chimirri, *J. Med. Chem.,* 2005, **48**, 7084;

   (c) I. Nicolaou and V. Demopoulos, *J. Med. Chem.,* 2003, **46**, 417;

   (d) J. E. Saxton, *Nat. Prod. Rep.,* 1997, **14**, 559;

   (e) M. Toyota and N. Ihara, *Nat. Prod. Rep.*, 1998, **15**, 327;

   (f) C.-C. Kuo, H.-P. Hsieh, W.-Y. Pan, C.-P. Chen, J.-P. Liou, S.-J. Lee, Y.-L. Chang, L.-T. Chen, C.-T. Chen and J.-Y Chang, *Cancer Res.,* 2004, **64**, 4621;

   (g) G. C. G. Pais, X. Zhang, C. Marchand, N. Neamati, K. Cowansage, E. S. Svarovskaia, V. K. Pathak, Y. Tang, M. Nicklaus, Y. Pommier and T. R. Burke, *J. Med. Chem.,* 2002, **45**, 3184.

Contributory Paper-82

Synthesis, characterization and the potential application of Co/Nd bimetallic nanoparticles-alumina nanoparticles @functionalized MWCNTs nanocomposite

Shreanshi Agrahari and Ida Tiwari*
Department of Chemistry (Centre of Advanced Study),
Institute of Science,
Banaras Hindu University,
Varanasi-221 005, India
E-mail: shreanshiagrahari@gmail.com (SA)
idatiwari@bhu.ac.in (IT)

Multiwalled carbon nanotubes (MWCNTs) has gained substantial significance from researchers owing to its attractive properties such as enormous surface area which acts as a supporting material with photocatalytic features, large thermal and chemical stability and better electrical conductivity. Moreover, MWCNTs has got several applications in polymer chemistry, light emitting diodes, gas discharge tubes, super capacitor, nanolithography, lithium ion batteries, fuel cells and electrochemical sensing. However, original MWCNTs may not be used in modification of electrode due to lack of solubility in water. Hence, functionalization of MWCNTs has been done to improves its dispersion in water, removes impurities from its surface and also useful in enhancing its electrochemical properties through fabrication with nanocomposites materials. Further, nanocomposite was synthesized using Co-Nd, alumina nanoparticles and fMWCNTs (Co-Nd@Al_2O_3-fMWCNTs) that not only acts as metal nanoparticles support but also enhanced its electro catalytic properties and increased sensitivity due to the synergistic effects of metal nanoparticles, alumina and fMWCNTs. Using several physicochemical characterization methods such as FT-IR, XRD, UV-visible studies, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and energy dispersive X-ray analysis (EDAX), the successful synthesis of the design nanocomposite material was verified. Glassy carbon electrode (GCE) modified with Co-Nd@Al_2O_3-fMWCNTs nanocomposite was used to prepare a sensitive electrochemical sensor for the determination of epinephrine (EP). Cyclic voltammetry response of the modified Co-Nd@Al_2O_3-fMWCNTs/GCE under optimal circumstances revealed a wide dynamic range between 0.2 to 14000 μM and LOD of 0.11 μM (S/N = 3). The designed sensor may be effective in measuring EP concentration in real biological samples.

Contributory Paper-83

Preparation of oxidized g-C_3N_4/CuAl-LDH nanocomposite as an advanced electrode modifying material for electrochemical sensing applications

Ankit Kumar Singh and Ida Tiwari*
Department of Chemistry (Centre of Advanced Study),
Institute of Science,
Banaras Hindu University,
Varanasi-221 005, India
E-mail: anksingh325@gmail.com (AKS)
idatiwari@bhu.ac.in (IT)

Recent research has shown that graphitic carbon nitride (g-C_3N_4), a stable allotrope in the carbon nitride family, is a promising candidate for a wide range of applications due to the availability of source materials, purity of composition, low cost, and ease of synthesis. Additionally, g-C_3N_4 has been widely used as a catalyst in light-emitting devices (LED), photocathodes, sensors, and imaging due to its distinct physicochemical properties, large surface area and abundant active sites and nanoarchitecture design. However, the poor electrical conductivity of g-C_3N_4 limits its applications in the field of electrochemical sensing. Hence, this study mainly based on improving the effective surface area and electrical conductivity of g-C_3N_4. The mixture of H_2SO_4-HNO_3-H_2O_2 was effectively used in the oxidation and exfoliation of the bulk graphite-like g-C_3N_4. Additionally, oxidized g-C_3N_4 and CuAl-LDH nanomaterials were combined together through simple mechanical mixing to prepare the hybrid nanomaterials. The prepared nanocomposite was thoroughly characterized using the proper analytical techniques. The physical characterizations were performed using FT-IR, XRD and XPS analysis while SEM and TEM analysis were used for morphological characterizations. The morphological and physico-chemical analysis proved that the oxidized g-C_3N_4/CuAl-LDH hybrid nanomaterial was successfully prepared. The newly synthesized oxidized g-C_3N_4/CuAl-LDH nanocomposite was drop casted on glassy carbon electrode and was successfully tested for electrochemical determination of diclofenac sodium (DS) to check its potential applicability in the field of electrochemical sensing. The Differential Pulse Voltammetry was employed for electrochemical sensing of DS in a wide detection range of 0.5–60 μM and detection limit as 0.38 μM. Further, the fabricated electrochemical sensor was effectively applied for the determination of DS in the prepared pharmaceutical formulation. Hence, these approaches intend to increase the practical usability of the prepared composite materials in the area of electrochemical sensing.

Contributory Paper-84

Light-induced reversible assembly of spiropyran functionalized gold nanoparticles and photoswithching of silicon surface potential

Mohammed Ikbal
Department of Chemistry,
Berhampore Girls' College (Affiliated to University of Kalyani),
Berhampore-742 101, Murshidabad, West Bengal, India
E-mail: md.ikbal.chem@gmail.com

Hybrid nanomaterials having tunable properties that can be reversibly conducted by external stimuli, in a particular light, are of great importance since they enable synergetic behaviour between their components and enable the design of stimuli responsive "smart" materials and surfaces. In this work we have described about the designed and synthesis of dithiolane-terminated T-shaped spiropyran derivative. Photophysical and photochromism of the free ligand was demonstrated. UV or visible light irradiation of gold nanoparticles (AuNPs) decorated with spiropyran, assist the reversible aggregation or dispersion of AuNPs. This process is accelerated by the electrostatic attraction/repulsion between the AuNPs controlled by the ring-opening (MC form)/ring-closing (SP form) photoisomerization reaction of the surface dyes. Moreover functionalized AuNPs modified smart silica surfaces were fabricated, where the concept of photoswitching is adapted to the surface by altering the contact potential with light irradiation.

Spiropyran derivatives are well-known photoswitchable molecules that undergo a reversible isomerization between two forms, having different properties. The colourless spiropyran consist of indoline and chromene moiety bound together via a spiro junction, perpendicular to one another gaining a three-dimensional orientation. This closed ring isomer absorbs at two wavelengths: at 270 nm the π–π^* electronic transition in the indoline part responsible for the absorbance and at 336 nm the band correlates with the chromene part of the molecule. UV irradiation on the hydrophobic SP isomer induces the opening of the ring generating the planar, zwitterionic and hydrophilic merocyanine (MC). Because of the π-conjugation between the indoline and the chromene moieties, MC possesses a delocalized single absorbance peak at the visible region giving MC a blue colour and a strong dipole moment. By the photoisomerization between these two states, a large and reversible change in the molecular properties can be achieved. This led to their uses in light-emitting diodes, molecular switches and molecular logic devices.

Contributory Paper-85

Study of corrosion inhibition efficiency of azole based drugs for mild steel in acidic medium

Rahul Mishra[a], Kanha Singh Tiwari[b], Chitrasen Gupta[a] and Shailendra Yadav[b]
[a]Department of Chemistry,
Kutir P.G. College, Chakkey,
Jaunpur-222 146, Uttar Pradesh, India
[b]Department of Chemistry,
Basic Science, AKS University,
Satna-485 001, Madhya Pradesh, India
E-mail: rahulmishra207966@gmail.com

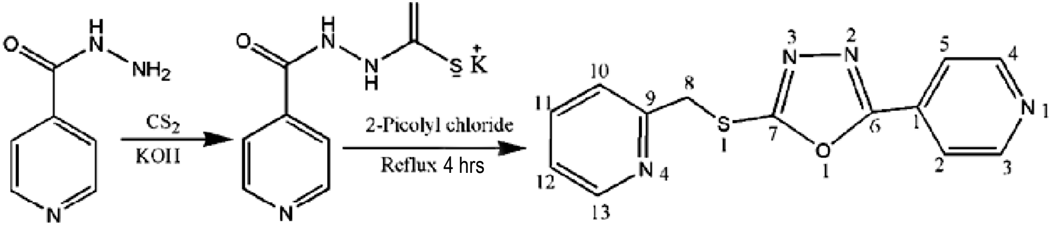
In industries prevention of metallic corrosion especially for closed systems appears as major issue. To resolve these issues various techniques are applied. Use of inhibitors is one of them and most of inhibitors are synthesized organic molecules containing N, S and O hetero atoms in their structures. Azole based drugs are being synthesized for their positive physiological effects and these compounds also contain S, O heteroatom with N heteroatom in their cyclic structure. Thus azoles based drugs have likely to inhibit corrosion of mild steel in acidic media. In present study, Teneligliptin, an azole based drug has been examined as corrosion inhibitor in fresh and expired form for mild steel in acidic medium (1N HCl) by using weight loss and electrochemical methods. Maximum inhibition efficiency 90 % was observed at 400 ppm concentration (30°C) for fresh drug. Expired drug exhibited 88% inhibition efficiency in similar conditions which is very close to fresh drug efficiency thus after expiry this drug can be utilized as cost-effective corrosion inhibitor.

Contributory Paper-86

Synthesis, fluorescence properties and electrochemical studies of 4-[5-(2-picolylsulfanyl)-1,3,4-oxadiazole-2-yl]-pyridine

Suryansh Chandra and Manoj Kumar Bharty
Department of Chemistry,
Institute of Science,
Banaras Hindu University,
Varanasi-221 005, India
E-mail: suryansh95chandra@gmail.com

1,3,4-Oxadiazoles have been used in a wide variety of biological applications and due to their excellent electron transport properties in the area of organic optoelectronic materials, which can be employed as two-photo absorption chromophores, second-order nonlinear optical materials and charge transfer materials in the organic light-emitting diodes they have gained considerate attention[1]. Numerous derivatives of 1,3,4-Oxadiazole displays strong fluorescence with high quantum yield and are used in the development of materials for electroluminescent devices and electron-transporting materials[2]. They have also been connected to chelating ligands in fluorescent complexes, to obtain emitting and charge transporting molecular species. Keeping the above facts in view, we have synthesized this new derivatives of oxadiazole 4-[5-(2-picolylsulfanyl)-1,3,4-oxadiazole-2-yl]-pyridine (pop). The synthesized compound pop has been characterized by elemental analyses, UV-vis., Infrared, NMR and X-ray diffraction data which crystallizes in a triclinic system having space group P-1. An electrochemical study shows that compound pop exhibits a reversible redox process assignable to a one-electron transfer reaction. Fluorescence spectra of Co^{2+}, Cr^{2+}, Cu^{2+}, Cd^{2+}, Hg^{2+} and Zn^{2+} ions with pop exhibit better fluorescence whereas Mn^{2+} and Ni^{2+} ions are less fluorescent as compared to the free pop. To get a better understanding of Frontier molecular orbitals and intramolecular charge transfer property, theoretical calculations,



Scheme 1. Synthesis of 4-[5-(2-picolylsulfanyl)-1,3,4-oxadiazole-2-yl]-pyridine (pop).

such as density functional theory (DFT), were performed which indicates that compound pop is soft and highly reactive.

References

1. P. Jayaprakash, M. Lydia Caroline, S. Sudha, R. Ravisankar, G. Vinitha, P. Ramesh and E. Raju, Synthesis, growth, optical and third-order nonlinear optical properties of L-phenylalanine D-mandelic acid single crystal for photonic device applications, *J. Mater. Sci. Mater. Electron*, 2020, **31**, 20460-20471.
2. A. P. Kulkarni, C. J. Tonzola, A. Babel and S. A. Jenekhe. Electron transport materials for organic light-emitting diodes. *Chemistry of Materials*, 2004, **16**, 4556-4573.

Contributory Paper-87

Noise-induced symmetry breaking of self-regulators: Nonequilibrium transition toward homochirality

R. Rafeek and D. Mondal
Department of Chemistry and Center for Molecular and
Optical Sciences & Technologies,
Indian Institute of Technology Tirupati,
Yerpedu-517 619, Andhra Pradesh, India
E-mail: rafna.rk@gmail.com

Studies on the origin of spontaneous chiral symmetry breaking in biomolecules have become a Holy Grail for chemists as it leads to a universal attribute of life, i.e., homochirality. In 1953, Frank provided a mathematical framework to explain a stable asymmetry from a symmetric mixture. He proposed that the origin of homochirality could be a consequence of an initial chiral bias in the reaction environment with autocatalytic growth and mutual antagonism. Subsequent variants of Frank's model support the fact that the stochastic nature of underlying reactions is efficient enough to generate an initial chiral seed. However, fluctuations in different reaction rates may lead to a nontrivial partially broken state during the chiral growth, i.e., a scalemic mixture. Upon altering the reaction condition, one partially broken chiral state can also undergo nonequilibrium transitions, leading to other optical states with different chiral symmetries.

In this study, we aim to rationalize a mechanism that explains the different upshots of chiral symmetry breaking and inspect the necessary condition for complete single-handedness. We consider a collection of Brownian particles, which can stay in any of the three possible isomeric states: achiral and enantiomers. Isomers are undergoing self-regulatory reactions along with chiral inhibition and achiral decay processes. The reaction rates of the isomeric states are guided by their neighbours and the thermal fluctuations of the system. We find that an alteration in the relative dominance of self-regulation, chiral inhibition, and achiral decay processes break the chiral symmetry of the system, which is either partial or complete. This results in four asymmetric population states: viz., three-isomer coexistence, enantiomeric coexistence, chiral–achiral coexistence, and homochiral state. We also report that fast stochastic self-regulation and a slow chiral inhibition and achiral decay process along with a threshold population of interacting neighbours suffice for the transition toward a complete symmetry broken state, i.e., homochirality.

References

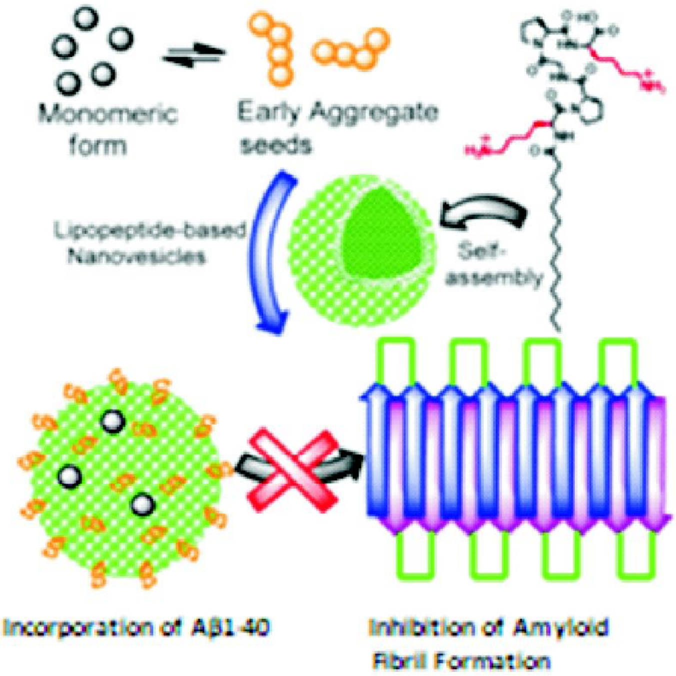
1. F. C. Frank, *Biochim. Biophys. Acta.,* 1953, **11**, 459.
2. G. Lente, *J. Phys. Chem. A,* 2004, **108**, 9475.
3. F. Jafarpour, T. Biancalani and N. Goldenfeld, *Phys. Rev. Lett.,* 2015, **115**, 158101.
4. R. Rafeek and D. Mondal, *J. Chem. Phys.,* 2021, **154**, 244906.

Contributory Paper-88

Self-assembling lipopeptide-based benign nanovesicles to inhibit amyloid fibril formation

Tapas Bera and Samit Guha*
Department of Chemistry, Organic Chemistry Section,
Jadavpur University,
Kolkata-700 032
E-mail: tapasbera2013@gmail.com

Alzheimer’s disease, a progressive severe neurodegenerative disorder, has been until now incurable, in spite of serious efforts worldwide. We have designed self-assembled myristoyl-KPGPK lipopeptide-based biocompatible nanovesicles, which can inhibit amyloid fibrillation made by the Aβ1-40 protein as well as reduce their neurotoxicity. Various spectroscopic and microscopic investigations illuminate that the lipopeptide-based nanovesicles dramatically inhibit random coil-to-β-sheet transformation of Aβ1-40. Förster resonance energy transfer (FRET) assay using synthesized Cy-3 (FRET donor) and Cy-5 (FRET acceptor)-conjugated Aβ1-40 also exhibits that nanovesicles strongly inhibit the fibril formation of Aβ1-40.



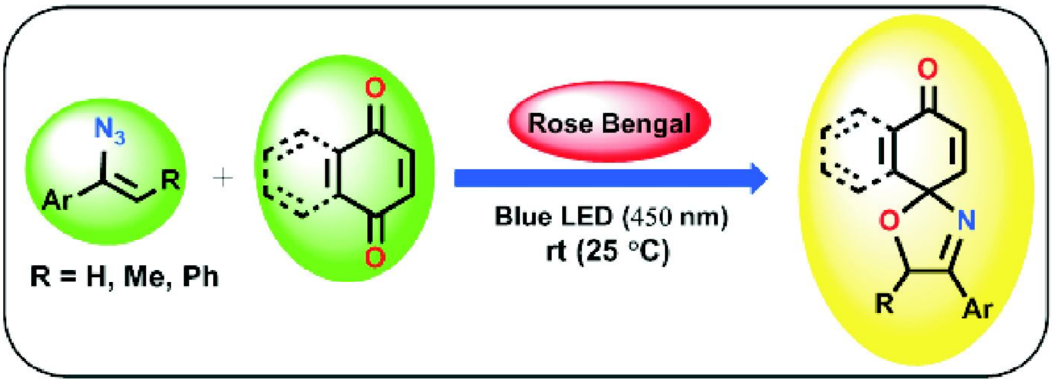
Schematic representation of the inhibition of amyloid formation of the Aβ1–40 by myristoyl KPGPK nanovesicles.

Contributory Paper-89

Visible-light-mediated synthesis of 1-Oxa-4-aza-spiro oxazolines by spiroannulation of quinones with vinyl azides

Subhankar Sarkar and Adinath Majee*
Department of Chemistry,
Siksha Bhavana,
Visva-Bharati
E-mail: sarkarsubhankar93@gmail.com

A new, simple and efficient method has been developed to synthesize 1-oxa-4-aza-spirooxazolines. The reaction was carried out at room temperature using rose bengal as an organic photoredox catalyst and blue LED as a light source. It was observed that quinones underwent spiroannulation reaction with vinyl azide on C-O double bond instead of C-C double bond through which various corresponding 1-oxa-4-aza-spirooxazolines have been synthesized in good to excellent yields.



References

1. A. De, S. Santra, A. Hajra, G. V. Zyryanov and A. Majee, *J. Org. Chem.,* 2019, **84**, 11735-11740.
2. A. De, S. Santra, G. V. Zyryanov and A. Majee, *Org. Lett.,* 2020, **22**, 3926-3930.
3. H. Xu, H. Tang, H. Feng and Y. Li, *Eur. J. Med. Chem.,* 2014, **73**, 46-55.
4. K. Weindel, S. Lewicka and P. Vecsei, *J. Steroid Biochem.,* 1989, **34**, 455-459.
5. W. Stegmann, P. Uebelhart and H. Heimgartner, *Helv. Chim. Acta,* 1983, **66**, 2252.

Contributory Paper-90

Designing and synthesis of a near infrared cy-PH switchable dye to target and image Lysosome

Ayan Mukherjee
Department of Chemistry,
Organic Chemistry Section,
Jadavpur University,
Kolkata
E-mail: ayan.mukherjee1964@gmail.com

Here, we have designed and synthesized acidic pH-activatable visible to NIR switchable ratiometric pH-sensitive fluorescent dye. The design consists of a cell-permeable organic probe containing a lysosome targeting morpholine functionality and an acidic pH-activatable oxazolidine moiety. The visible closed oxazolidine form (λabs 418 nm) can be switched to the highly conjugated NIR Cy-7 form (λabs 780 nm) through ring opening of the oxazolidine moiety at acidic pH. This switching of the ratiometric fluorescent probe is highly reversible and can be controlled by pH. NMR, UV/vis and fluorescence spectroscopies allowed monitoring of pH switching behavior of the probe. This bioresponsive *in situ* acidic organelle activatable fluorophore showed reversible pH-switchable ratiometric optical properties, high photostability, huge bathochromic emission shift of 320 nm from basic to acidic pH, off-to-on narrow NIR absorption and emission bands with enhanced molar extinction coefficient at lysosomal pH, good quantum yield, low cytotoxicity, and targeted imaging ability of live cell lysosomes with ideal pKa. The report demonstrated ratiometric imaging with improved specificity of the acidic lysosome while minimizing signals at the NIR region from nontargeted neutral or basic organelles in human carcinoma HeLa and A549 as well as rat healthy H9c2(2-1) live cells, which is monitored by confocal laser scanning microscopy.

Contributory Paper-91

High entropy effect on magnetic properties of double perovskite: La_2MnCoO_6

Radhamadhab Das
Visva-Bharati University
Santiniketan-731 235
E-mail: rmdaschem@gmail.com

The main work of my presentation is based on synthesis, structure and magnetic properties of La_2MnCoO_6 and the high entropy stabilized $(La_{0.4}Y_{0.4}Ca_{0.4}Sr_{0.4}Ba_{0.4})MnCoO_6$. The main characterization of this samples have been done by using P-XRD, TEM, ED, EDX. Energy Dispersive X-Ray together with high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) confirms the chemical homogenity of La_2MnCoO_6 and the high entropy oxide phase i.e. $(La_{0.4}Y_{0.4}Ca_{0.4}Sr_{0.4}Ba_{0.4})MnCoO_6$. The structural symmetry of La_2MnCoO_6 and $(La_{0.4}Y_{0.4}Ca_{0.4}Sr_{0.4}Ba_{0.4})MnCoO_6$ are orthorhombic and cubic respectively which confirms from P-XRD and ED studies. The high temperature magnetic ordering at T_C~225 K expected for an atomically ordered La_2MnCoO_6 is suppressed in the corresponding quenched sample. The atomic disordering in quenched La_2MnCoO_6 results in coexistence of the phases where vibronic ferromagnetism and antiferromagnetic states appeared at T_C~ 135 K and T_N~ 150 K, respectively. Whereas the high entropy stabilized $(La_{0.4}Y_{0.4}Ca_{0.4}Sr_{0.4}Ba_{0.4})MnCoO_6$ exhibits antiferromagnetic transition at T_N~ 150 K and low temperature magnetic frustration at 45 K and 15 K due to localized competing interactions. The drastic suppression of ferromagnetic state in $(La_{0.4}Y_{0.4}Ca_{0.4}Sr_{0.4}Ba_{0.4})MnCoO_6$ suggests that the essential interaction is of antiferromagnetic nature in cationically disordered La_2MnCoO_6 perovskite. We have suggested that the size disorder parameter, σ^2 plays a significant role in determining the magnetic ground state of the high entropy stabilized perovskite.

Contributory Paper-92

Solar energy conversion and storage through the Photogalvanic cells: A perspective

Reetoo* and Pooran Koli#
Department of Chemistry, Faculty of Science,
Jai Narain Vyas University,
Jodhpur-342 033, Rajasthan, India
E-mail: reetooraani86@gmail.com

The photo galvanic cells (PG) are electrochemical devices enabling solar energy conversion and storage. The PG cells are based on the liquid phase electrolyte (containing sensitizer, reductant, surfactant and alkali) in which two electrodes (working and counter electrodes) are dipped[1]. The mechanism of photocurrent generation in PG cells involves various photo-physical processes like photon absorption, formation of excited states of the sensitizer molecules, reduction of excited sensitizer molecule, and electron migration from sensitizer to working electrode to external circuit to counter electrode. The main fabrication components of the PG cells are as sensitizer, reductant, surfactant, alkali, electrodes, cell vessel, etc. Over the years, the scientists have focused on these components for further improvement of the PG cells. A study is reported on the effects of various operating parameters on the electrical output of the Bromophenol Red photosensitizer-EDTA reductant based PG cells[2]. The synthesis of sodium 4-dodecyl benzene sulfonate anionic surfactant from petroleum waste through two steps method and consequently its use in PG cells is also reported[3].

PG cells (original dye based solar cell) have yet to fulfill their promise as a low fabrication cost with scalable energy conversion system. The efficient performance of PG cells relies on high dye solubility and selective electrodes with fast electron transfer kinetics. Instead of illuminating the device through the electrode (conventional approach), a new vertical configuration is employed with light coming between the two electrodes. This way the light absorption and hence electron generation spreading through the depth of the device no longer requires unreasonably fast electrode kinetics. The readily available Thionine-Iron dye-mediator couple could achieve 6 % efficiency if highly selective electrodes are used, compared to 0.45 % at best using the conventional approach. It is suggested that upon the realization of highly selective electrodes and an improved dye/mediator couple, the efficiency of ≥ 13 % can be achieved from the new configuration[4]. Dye-surfactant interaction in aqueous solutions is important in dyeing and electrochemical devices like solar cells[5]. The dye-surfactant complex having greater stability in excited state might be more useful for improvement the PG cells[6].

There are various challenges like, dye decay, hampering of efficiency by back electron transfer, sacrificial nature of the organic reductant, water solvent evaporation, metal electrode rusting, low efficiency, etc., facing the PG cells. The PG cells reported so far involves liquid phase electrolyte and the stability of liquid phase electrolytes is low in comparison to that of solid-phase solar cells. The technique of emission loss using the luminescent solar spectrum splitter design, single-layer graphene/Cu_2S nanocomposite counter electrode, carbon counter electrode, phthalocyanines sensitizers, the cobalt phthalocyanine sensitized $SnIn_4S_8$/g-C_3N_4 composites and chemically modified amino phthalocyanine-GPTMS/TiO_2 may be used to further improve the PG cells[7]. Therefore, the future research in the area of photogalvanics should focus on these challenges. These cells are capable of solar power generation at low cost with inherent storage capacity. Therefore, this property of PG cells needs to be exploited as this technology is cleaner and promising for application in daily life.

References

1. *Int. J. Res. Applied Sci. Eng. Tech.*, 2018, **6(3)**, p.2321.
2. *J. Power Sources.,* 2006, **159(1)**, p.747.
3. *J. Mol. Struct.*, 2021, **1243**, p.130764.
4. *Electrochimica Acta*, 2014, **143**, p.98.
5. *Energy Reports,* 2018, **4**, p.23.
6. *J. Saudi Chem. Soc.*, 2019, **23(1)**, p.83.
7. *Bioresources Tech. Reports,* 2022, **18**, p.101083.

Contributory Paper-93

Template-directed shape control synthesis of rare earth sulfide for electrochemical water splitting

Arti Maurya and Mahendra Yadav*
Department of Chemistry and Chemical Biology,
Indian Institute of Technology (Indian School of Mines)
Dhanbad, Jharkhand-826 004, India
E-mail: mahendra@iitism.ac.in

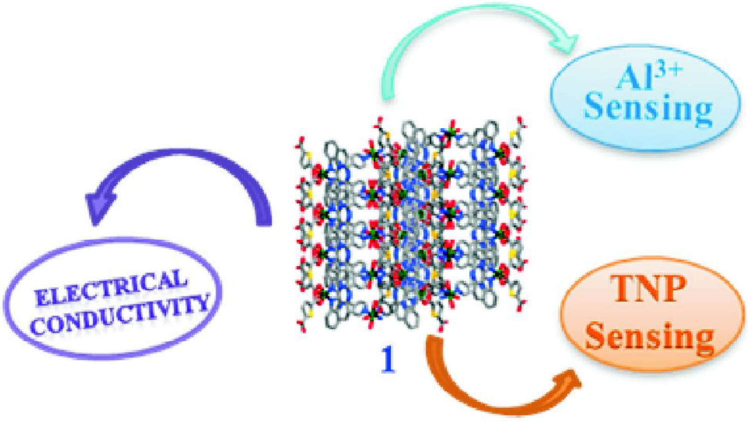
Increasing energy demand, and widespread concern about the global warming and impending the global energy crisis due to the overuse of the fossil fuel prompting the urgent need of the alternative energy source. In this way electrochemical water splitting is the one of the convenient and environment friendly for a hydrogen economy. Water splitting process is consist of the two half-cell reactions cathodic hydrogen evolution reaction (HER) and the anodic oxygen evolution reaction (OER). However oxygen evolution process is the sluggish kinetics and the required very high Overpotential. It occurs by the complex mechanism, four electron proton coupled process, which greatly reduces the water splitting efficiency. Therefore, extensive research has been performed for the alternative class of electrocatalyst for the OER to compete the extensive benchmark IrO_2 and RuO_2 catalysts. These noble metal oxides are inadequacy and high cost limits it for industrial application as the energy conversion. Herein we synthesized Template – Directed Shape Control Synthesis of Rare Earth Sulfide for water splitting as Oxygen Evolution Reaction (OER), which show the significant low over potential in the alkaline medium. The synthesized material is confirmed by different techniques like X-ray diffraction (XRD), Field emission scanning electron microscope (FESEM), High-resolution Transmission electron microscope (HRTEM), selected area electron diffraction (SAED), Energy-dispersive X-ray (EDX), X-ray Photoelectron spectroscopy (XPS) and different electrochemical study for the show the application of synthesized material. The prepared sample is used as a bi-functional electrocatalyst towards HER and OER.

Contributory Paper-94

Synthesis of amultifunctional 3D Zn(II)-MOF based on pyridyl-imidazoquinazoline: Structure, luminescence, selective and sensitive detection of Al^{3+} and TNP, and its semiconducting device application

Gurupada Bairy and Chittaranjan Sinha*
Department of Chemistry,
Jadavpur University,
Kolkata-700 032, India
E-mail: gurupadabairy@gmail.com

At the age of sustainable development, exploration of multifunctional materials is of high priority for their economic benefits and environmental suitability. A stable luminescent coordination polymer, $[Zn_2(\mathbf{tdc})_4(\mathbf{pdiq})_3]$ (**1**), (**pdiq** = pyridyl-imidazoquinazoline; $\mathbf{H_2tdc}$ = 2,5-thiophenedicarboxylic acid) has been prepared and structurally confirmed by the single crystal X-ray diffraction analysis. The 3D framework consists of distorted octahedral geometry with ZnO_4N_2 coordination sphere where four carboxylato-O donations come from two $\mathbf{tdc}^{2-}$ as bridging ligand and two pyridyl-Ns from two **pdiq**. The $\pi\cdots\pi$ interactions between imidazolium and phenyl groups bestow robustness to the architecture. High dispersibility of Zn-MOF (**1**) in acetonitrile may enhance the fluorescence intensity than water that has prompted for fluorescence measurements in the former solvent and is used for efficient and selective turn-off ratiometric sensing of Al^{3+} ions (LOD, 1.39×10^{-7} *M*). In addition, the fluorescence emission of **1** is instantly quenched by trinitrophenol (TNP) and the LOD is 1.54×10^{-7} *M*. The Tauc's plot measures the semiconducting band gap (3.33 eV) and the electrical conductivity is significantly increased upon illumination (Λ: 1.14×10^{-3} S m^{-1} (dark), 5.35×10^{-3} S m^{-1} (light)) and that the energy barrier declines marginally (FB: 0.57 (dark), 0.49



(light)). Transit time (τ) and diffusion length ($\boldsymbol{L_D}$) at the quasi-Fermi level have been analyzed to offer information on the charge transport mechanism of the compound. The better performance on photo-irradiation signifies enhanced charge transfer kinetics of Zn-MOF coated Thin-Film Device (**TFD 1**) which encourages its application in semiconductor devices.

Contributory Paper-95

Ionic species recognition using a derivative of rhodamine as a sensor

Amit Kumar Chaturwedi and Milan Hait*
Department of Chemistry,
Dr. C.V. Raman University,
Kargi Road, Kota,
Bilaspur-495 113, Chhattisgarh, India
E-mail: amitchaturwedi1@gmail.com
haitmilan@gmail.com

The trivalent of chromium cation (Cr^{3+}) and fluoride anion (F^-) was recognized by using the rhodamine urea methacrylate-based fluorescent probe (RhBUA) and its consequent cationic complex are also described. Then on-fluorescent rhodamine derivatives can recognize Cr^{3+} ion over other included metal ions in CH_3CN-H_2O (90/10v/v) at neutral pH solutions with a 1:1 stoichiometry. This precise conditions can lead to a prominent fluorescence OFF-ON switching response of synthesized chemosensor probe.

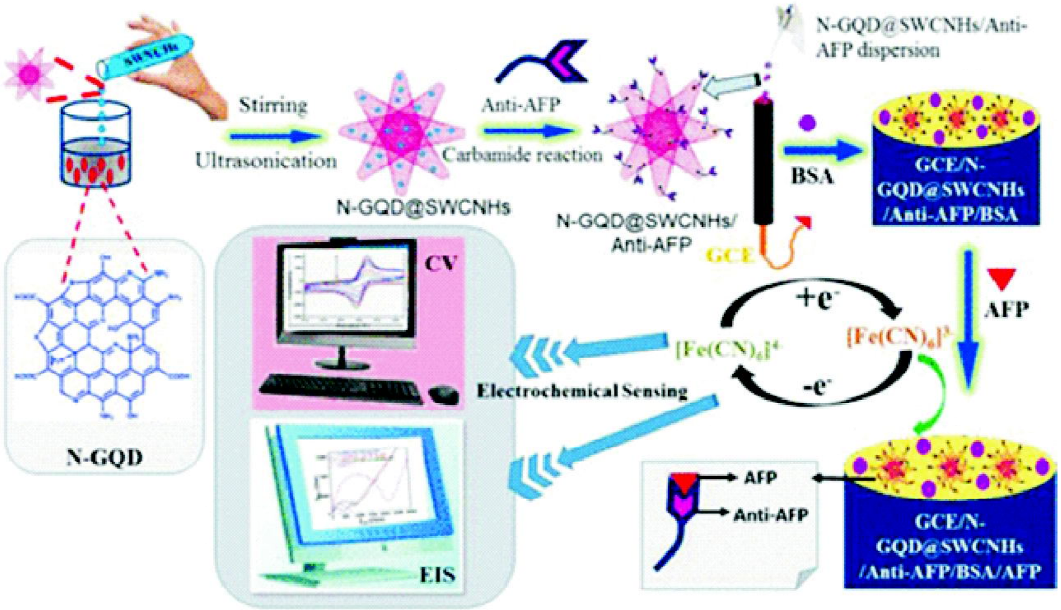
This research work observed that rhodamine derivative and chromium ion complex i.e. (RhBUA-Cr^{3+}) can consequently serve as a chemosensor and detect selectively fluoride (F^-) ion. A complete signal quenching (fluorescence ON-OFF switching) phenomenonal mechanism is studied in this research work. This fluorescence ON-OFF switching mechanism can happen due to Cr^{3+} cation extraction and the resulting deformation of RhBUA-Cr^{3+} complex.

Contributory Paper-96

Development of an efficient immunosensing platform by exploring single-walled carbon nanohorns (SWCNHs) and nitrogen doped graphene quantum dot (N-GQD) nanocomposite for early detection of cancer biomarker

Adrija Ghosh
University of Calcutta, Rajabazar,
Kolkata
E-mail: adrijaghosh1996@gmail.com

In this work, a novel electrochemical immunosensor based on nitrogen doped graphene quantum dot (N-GQD) and single-walled carbon nanohorns (SWCNHs) was developed for the detection of α-fetoprotein (AFP), a cancer biomarker. Thus, to fabricate the platform of the immunosensor, nanocomposite architecture was developed by decorating N-GQD on the surface of the SWCNHs. The resulting hybrid architecture (N-GQD@SWCNHs) functioned as an exceptional base for the immobilization of antibody (Anti-AFP) through carbodiimide reaction with good stability and bioactivity. The immunosensor was prepared by evenly distributing the bioconjugates (N-GQD@SWCNHs/Anti-AFP) dispersion on the surface of the glassy carbon electrode and subsequently blocking the remaining active sites by bovine serum albumin to prevent the nonspecific adsorption. Cyclic voltammetry and electrochemical



impedance spectroscopy technique was employed to investigate the assembly process of the immunosensor. Under optimal conditions, the immunosensor exhibited a broad dynamic range in between 0.001 ng/mL to 200 ng/mL and a low detection limit of 0.25 pg/mL. Furthermore, the sensor showed high selectivity, desirable stability, and reproducibility. Measurements of AFP in human serum gave outstanding recovery within 99.2% and 102.1%. Thus, this investigation and the amplification strategy exhibited a potential role of the developed nanocomposite based sensor for early clinical screening of cancer biomarkers.

Contributory Paper-97

Synthesis, characterization and understanding of agar based ON-OFF-ON fluorescent probe

Debrupa Biswas
Polymer & Nano Research Laboratory,
Department of Chemistry,
Siksha-Bhavana, Visva-Bharati University,
Santiniketan-731 235, India
E-mail: debrupab56@gmail.com

A fluorescent dye functionalized polymer with enhanced aqueous solubility and biocompatibility has been synthesized via single step condensation reaction of 1-pyrenecarbaxaldehyde with agar. The synthesized fluorescent probe is characterized by NMR, PXRD, SEM, FTIR, absorption and emission spectra to develop an effective probe. The quantum yield of the probe is sufficiently high (0.025), which is suitable for the sequential detection of Fe^{3+} and F^{-} through 'ON-OFF-ON' fluorescence response technique. These unique optical responses have been effectively utilized to construct a polymeric logic gate where Fe^{3+} and F^{-} act as chemical inputs and emission at 469 nm as the desired output. An attempt has been made to understand the optical behavior of the probe in the light of theoretical studies (DFT, FMO). The quenching behavior of the synthesized probe has been explained through chelation enhanced quenching (CHEQ). Also, the probe has been used to detect vitamin C.

Contributory Paper-98

Effect of nickel doping on magnetic properties in Swedenborgite type "114" cobaltite

Sudipa Bhattacharya
Department of Chemistry,
Siksha-Bhavana, Visva-Bharati University,
Santiniketan-731 235, West Bengal, India
E-mail: bhattacharya.sudipa82@gmail.com

Co- based homologues of the mineral swedenborgite exhibits not only the oxygen storage capacity but rich varieties of magnetic properties and ground states. The Ca-based "114" cobaltite, $CaBaCo_4O_7$ is unique in that it is the only member of this family which exhibits a ferromagnetic ground state at a low temperature ($T_C = 60$ K). The unique magnetic behaviour of $CaBaCo_4O_7$ is rooted out from the non-collinear arrangement of the cobalt spins which form ferromagnetic Co^{2+} zig-zag chains running along the *b* direction. In this presentation , I will discuss the effect of tiny Ni-doping in swedenborgite type cobaltite $CaBaCo_4O_7$. Ni-doping in ferrimagnetic $CaBaCo_4O_7$ slightly reduce the orthorhombic distortion and no structural transition is observed for the doping range ($0 < x \leq 0.07$). The overall structural distortion is only 0.018% for x = 0.07. A significant change in magnetic properties of $CaBaCo_{4-x}NixO_7$ ($0 \leq x \leq 0.07$) is observed just with 0.5% Ni-doping. The dramatic suppression of ferrimagnetic state of $CaBaCo_4O_7$ avobe 1% doping suggests the sensitivity of Ni-doping on magnetic properties of $CaBaCo_4O_7$. By compairing the result with other reported Co-site doping in $CaBaCo_4O_7$ we have suggested an explanation of exceptional sensitivity of Ni-doping. Ni-doping results in competing magnetic phases, ferrimagnetic phase, an antiferromagnetic phase, metamagnetic phase and magnetic frustration at lower temperature. We observed a decrease in ferrimagnetic TC and the remanent magnetization(Mr) value drastically decrease with increasing Ni-doping level in $CaBaCo_{4-x}NixO_7$ ($0 \leq x \leq 0.07$). The successive replacement of Co^{2+} by magnetic Ni^{2+} in the zig-zag ferromagnetic chain in kagome layer puturbs the magnetic interaction through antiferromagnetic exchange with cobalt spins following Goodenough-Kanamori rules. This possibly reorient the cobalt spin adjacent to the dopant which strongly modifies ferromagnetic ground state resulting competing magnetic states. These are responsible for the change in magnetic ground state of $CaBaCo_4O_7$ which results in suppression of ferrimagnetic state with the evolution of antiferromagnetism and magnetic frustration.

Contributory Paper-99

Critical understanding of metal-guided photochromism

Nandagopal Bar and Pranesh Chowdhury*
Polymer & Nano Research Laboratory,
Department of Chemistry,
Siksha Bhavana, Visva-Bharati University,
Santiniketan-731 235, India
E-mail: nandagopalbar1995@gmail.com
pranesh.chowdhury@visva-bharati.ac.in
pranesh_02@yahoo.co.in

Dye containing Schiff base metal-complex is a new member of the photochromic family with advantages such as long-wavelength absorption, high molar absorption coefficient, large Stokes shift, facile synthesis, good photoresponse and excellent fatigue resistance. The system is highly promising for the fabrication of simple devices like photoprinting, photopatterning, UV light sensing, etc. In this work, an excellent metal-guided photochromic (MG-PC) material is synthesized using Rhodamine B hydrazide, trihydroxybenzaldehyde and Zn^{2+} via Schiff base chemistry with a view to construct a molecular keypad lock. All the issues related to photochromism (photophysical properties, kinetics, thermodynamics, photostationary state, quantum yield, fatigue resistance and effect of various controlling factors) have been understood and tuned accordingly to achieve the target of quick responsive MG-PC system. The significantly low activation energy (E_a = 27.53 kJ/mol) for the thermal bleaching justifies the achievement of target. The MG-PC material involves photo-tautomerism (PT), which is consist of photo-colouration (conversion of pale green-yellow enol to pink colour keto form exclusively under UV-light) and thermal bleaching (return back to original enol form under dark below the critical temperature, 50°C). The PT proceeds through metal-guided excited state and ground state intramolecular proton transfer as evident from the large Stokes shift (λ_{ex} = 365 nm, λ_{em} = 581 nm). The theoretical analyses (DFT, TD-DFT, PES, FMO, etc.) provide a deep insight into the mechanistic aspects and helps in understanding the experimental evidences. The present work attempts to solve the long-standing problem associated with the mechanistic path (the passage of proton transfer, transition states, FMO, etc.) involves in the photochromism. The photo-responsiveness is categorised firmly for the first time as photo-thermal reversible process (T-type). The developed system demonstrates large scope to design molecular logic gates and keypad lock.

Contributory Paper-100

A novel Schiff base based optical probe for the detection of Zn^{2+} ions

Swapan Kumar Mazumder and Pranesh Chowdhury*
Department of Chemistry,
Siksha-bhavana, Visvabharati University,
Santiniketan-731 235, India
E-mail: mazumder.swapankumar@gmail.com
pranesh.chowdhury@visva-bharati.ac.in
pranesh_02@yahoo.co.in

A new Schiff base is designed and synthesised using amine derivative of toluene and an aromatic aldehyde. An analytical method has been developed to detect Zn^{2+} in methanol solution using the synthesised Schiff base. The emission intensity of the solution of Schiff base was gradually enhanced due to addition of methanol solution of Zn^{2+}. The observation can be explained by chelation enhanced fluorescence (CHEF) process. The detection limit of probe was found very low, concluded through the spectrophotometric titration method. Not only this, the synthesised probe works glowing in physiological pH range. Thus this could be employed for the estimation of Zn^{2+} qualitative as well as quantitative.

$$\text{A mine derivative of Tolunene} \xrightarrow[\text{Methanol}]{\text{Aromatic aldehyde}} \text{Schiff base (non fluorescent)} \xrightarrow[\text{(Turn on through CHEF)}]{Zn^{2+}} \text{Green fluorescence}$$

Contributory Paper-101

Characterisation of Au_{20} nanocluster for biomedical applications

Nineesha Sen Banerjee[a,b] and Madhurima Chakraborty[a]
[a]Department of Biochemistry,
West Bengal State University
[b]Department of Biochemistry,
Vivekenanda College
E-mail: nineesha99@gmail.com

Small gold clusters for a long while have gained the interests of modern nanotechnologists. Electronic and geometric structures are being determined to study the distinct catalytic and binding property of such clusters which will build a perception of a molecular model of gold nano clusters in theoretical research. Au_{20} magic cluster has been chosen as out of such clusters, as it has the inherent properties of a magic metal cluster and its size is near the fermi wavelength of an electron in bulk gold. The stability and symmetric geometry of atomically defined Au_{20}, make it paradigm for study based on gold surface interaction. DFT calculations of the concerned cluster reveals in having a tetrahedral structure with a hollow centre and all the twenty atoms lying on the surface of the four faces. Au_{20} nanocluster consisting of four atoms on the apex, at the centre and twelve at the edges. A bond distance of ~2.79 – 2.8 Å between the adjacent apical atoms, ~2.91 Å at the centre of the faces of nearby atoms, ~2.73 Å and ~3.1 Å among the edge atoms and between the edge and apical atoms respectively is obtained on optimising the structure. To conclude, Au_{20} acts as an architype of gold nanoparticles, with its variation in coordination environment offering surface sites for binding biological molecules which may be used for prospective biomedical applications.

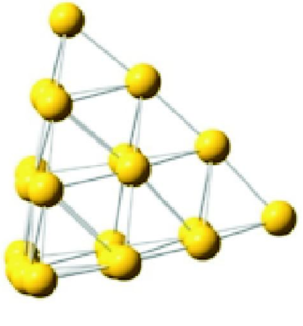


Fig. 1. Tetrahedral structure of optimised Au_{20} nanocluster.

Contributory Paper-102

Facile synthesis of rhodamine B salicylaldehyde hydrazone chemosensor: Colorimetric and fluorometric detection of Cu^{2+} ion

Arindam Ray and Pranesh Chowdhury*
Polymer & Nano Research Laboratory,
Department of Chemistry,
Siksha Bhavana, Visva-Bharati University,
Santiniketan-731 235, India
E-mail: arindamray223@gmail.com
pranesh.chowdhury@visva-bharati.ac.in

A new dye-containing Schiff-base of rhodamine B salicylaldehyde hydrazone was designed and facilely synthesized from rhodamine B by a two-step reaction. This Shiff base was stable in neutral water solutions for at least 2 days. It was designed to chelate with metal ions via its carbonyl O, imino N and phenol O atoms. The spirolactam moiety of the rhodamine group acted as a signal switcher, which was envisioned to turn on when the cation was bound. The newly developed Schiff-base displayed a reversible absorption and fluorescence enhancement response to Cu(II) via a 1:1 binding mode. Its selectivity toward Cu(II) is very high because little interference was observed for other commonly coexistent metal ions. The detection of Cu(II) by the Schiff-base at a lower micromolar level was successful even in buffered water.

Contributory Paper-103

Design and synthesis of imine based metal free organocatalyst for conversion of isocyanates to urea derivatives

Mainak Sarkar, P. Chakrabortty and Sk. Manirul Islam*
Department of Chemistry,
University of Kalyani, Kalyani,
Nadia-741 235, West Bengal, India
E-mail: ami.mainak1997@gmail.com
manir65@rediffmail.com

Catalysis plays a significant role in the growing demand for industrial processes. Photocatalytic synthesis of urea derivatives from a wide range of isocyanates was demonstrated under inert atmosphere using the mesoporous Covalent Organic Framework (COF) under visible light[1]. Application of covalent organic framework-based catalysts has received great attention in recent years due to their potential advantages over the homogeneous ones[2,3]. The present work consists of synthesis, characterization and catalytic evaluation of a new two-dimensional porous metal free covalent organic frameworks (PHTA) with imine linkers and their applications in synthesis of urea. These catalysts have been characterized by powder XRD, TEM, EDX, FT-IR, EPR, BET, XPS, SEM-EDX, UV-vis spectral studies and thermo gravimetric analysis[4,5].

Good catalytic activity and efficiency of these catalysts suggest that the present catalytic systems would be useful to synthesize industrially important fine chemicals.

References

1. P. Chakrabortty, S. Biswas, A. Das, M. Dolai and S. M. Islam, *Molecular Catalysis,* 2022, **522**, 11213.
2. S. Ghosh, R. A. Molla, U. Kayal, A. Bhaumik and S. M. Islam, *Dalton Transaction,* 2019, **48**, 4657-4666.
3. M. Halder, Md. M. Islam, Z. Ansari, S. Ahammed, K. Sen and S. M. Islam, *ACS Sustainable Chemistry* & Engineering*,* 2017, **5**, 648.
4. R. A. Molla, M. A. Iqubal, K. Ghosh and S. M. Islam, *Green Chemistry.* 2016, **18**, 4649.
5. S. Roy, P. Bhanja, A. Bhaumik and Sk. Manirul Islam, *Chemical Communications,* 2016, **52**, 1871.

Contributory Paper-104

Two dimensional $Ti_3C_2T_X$ MXene nanosheets for electrochemical carbon dioxide reduction into multi-carbon products in aqeuous medium

Sarathkumar K. and Dhirendra K. Rai*
Sustainable Energy & Environmental Materials Lab,
Department of Metallurgy Engineering and Materials Science,
Indian Institute of Technology Indore,
Simrol-453 552, Madhyapradesh
E-mail: phd1701205012@iiti.ac.in

In the present era, rapid industrial growth and energy production emancipate most of the green house gases in the environment. Among different gases, continuous emission of carbon dioxide (CO_2) to the environment leads to adverse effects on the entire ecosystem. As per the Mauna-Loa observatory, the present CO_2 level is ~416 ppm in the atmosphere; the increase in the concentration of CO_2 in every year consequences global warming. Therefore, it is imperative to explore novel and efficient strategies for capturing and converting CO_2 into valuable synthons.

In this work, two-dimensional (2D) $Ti_3C_2T_X$ MXene has been successfully synthesized by a top-down approach, involving selective etching of the Aluminium layer from the parent titanium MAX phase (Ti_3AlC_2) to yield the MXene nanosheets. The structural and morphological characteristics of the as-prepared $Ti_3C_2T_X$ MXene have been characterized by powder X-ray diffraction, Raman spectroscopy, and field-emission scanning electron microscopy. CO_2 adsorption studies have been carried out using BET surface adsorption analyser. Electrocatalytic CO_2 reduction properties on the prepared MXene are evaluated using a conventional three-electrode system.

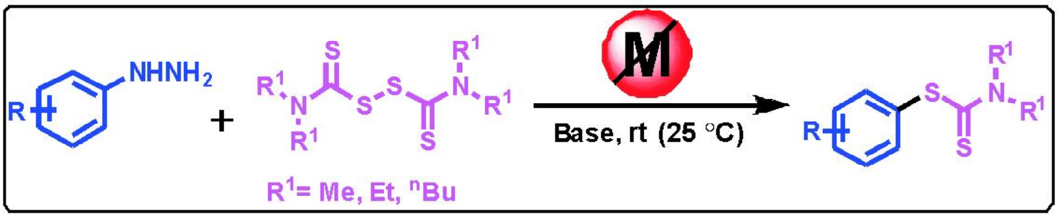
Various physical characterizations have confirmed the successful formation of $Ti_3C_2T_X$ MXene. The CO_2 capture studies reveal that the prepared adsorbent has the maximum adsorption capacity of 0.16 mmol/g at 298 K and 1 atm pressure. The presence of Ti metal centres in the adsorbent favours the CO_2 adsorption through physisorption, which is supported by low enthalpy of adsorption of –29 kJ/mol. Contrary to previous CO_2 electro reduction in organic electrolytes, the present electrocatalyst exhibits more than 50% of faradaic efficiency for the formation of C_{2+} production in environmentally benign aqueous system. Mechanistic investigation using Tafel's plots shows single electron transfer is the rate-determining step for product formation. Moreover, the catalyst features excellent stability for product formation. This excellent electrocatalytic performance is the consequence of its superior conductivity and the presence of Ti metal centres. Thus, this study can provide a positive impact on the development of Ti-based earth-abundant catalyst for C_{2+} product formation in simple aqueous electrolytes.

Contributory Paper-105

Metal-free synthesis of aryl dithiocarbamates via C(sp^2)–S coupling reactions of arylhydrazine with thiuram disulfide reagents

Satyajit Pal and Adinath Majee*
Department of Chemistry,
Siksha Bhavana,
Visva-Bharati
E-mail: palsatyajit18@gmail.com

A metal-free, environment-friendly and efficient protocol of C(sp^2)–S coupling reaction of arylhydrazine and low-cost tetraalkylthiuram disulfides was developed for the synthesis of aryl dithiocarbamates. The themes of our developed method were catalyst-free, mild reaction conditions, room temperature synthesis with high yields, and broad substrate scope. Apart from this, our approach is also helpful for synthesizing potentially bioactive compounds and drug modification.



References

1. S. Sarkar, S. Santra, G. V. Zyryanov and A. Majee, *ACS Sustainable Chem. Eng.,* 2021, **9**, 16, 5557-5569.
2. S. Pal, R. Chatterjee, S. Santra, G. V. Zyryanov and A. Majee, *Adv. Synth. Catal.,* 2021, **363**, 1-11.
3. Y. Shieh, K. Du and C. Lee, *J. Org. Chem.,* 2019, **84**, 10, 6223-6231.
4. G. Kibriya, S. Mondal and A. Hajra, *Org. Lett.,* 2018, **20**, 23, 7740-7743.
5. Z. Dong, X. Liu and C. Bolm, *Org. Lett.,* 2017, **19**, 21, 5916-5919.
6. D. Kundu, S. Ahammed and B. C. Ranu, *Org. Lett.,* 2014, **16**, 6, 1814-1817.

Contributory Paper-106

Preparation of magnetic nanoparticles

Shreya Chatterjee
Jadavpur University, Jadavpur,
Kolkata, West Bengal
E-mail: shreyachatterjeeblp@gmail.com

With the advancement in drug delivery system it has always been a challenge to the researchers for the formulation to a type of drug delivery system which will have less toxicity, targeted delivery and will be highly biodegradable. Nano science or nanotechnology have proved to be an effective way of targeting the drug to its active site because of its unique physicochemical properties and size thereby reducing the dose of administration, increasing bioavailability and also reducing toxicity.

Magnetic nanoparticles in recently few decades have proved to be an effective drug delivery system due to its high magnetic responsiveness, biocompatibility, high targeted drug delivery efficiency etc. The drug can be easily targeted to the active site by the application to a magnetic field applied externally. Among the various elements, nanoparticles prepared with iron oxide/iron oxide nanoparticles are widely used due to its high electrical resistivity, mechanical hardness, chemical stability etc.

Magnetite nanoparticles (Fe_3O_4) was synthesized by a simple co-precipitation method using aqueous salts of anhydrous Ferric chloride anhydrous ($FeCl_3$) and Iron(II) SulphateHepta Hydrate ($FeSO_4.7H_20$) in various ratios in 5 different formulations by using sodium hydroxide (NaOH) as a base and maintaining a constant temperature of about 70–80°C and stirring speed of about 600–700 rpm. The black precipitate obtained was filtered; dried and magnetic nanoparticles were obtained. The magnetic nanoparticles obtained were further characterized by XRD, SEM and EDAX analysis. XRD graph for formulation P1 clearly showed the peak for the presence of magnetic nanoparticle. SEM images for formulation P1 showed spherical particles and EDAX spectra presented strong Fe and O. Formulation P1 is regarded as best formulation as per the XRD data obtained for 5 formulations. Overall it can be concluded that magnetic nanoparticles were synthesized and characterized accurately.

Contributory Paper-107

Response of a newly developed Schiff base chemosensor with selective Zn(II) and Ni(II) sensing efficacy via turn-on fluorescence response results to a mononuclear Zn(II)/Ni(II) complex having ATP detection ability in aqueous medium

Shubham Ray and Tithi Maity*
Department of Chemistry,
Prabhat Kumar College, Contai,
Contai, Purba Medinipur
E-mail: shubham.info94@gmail.com

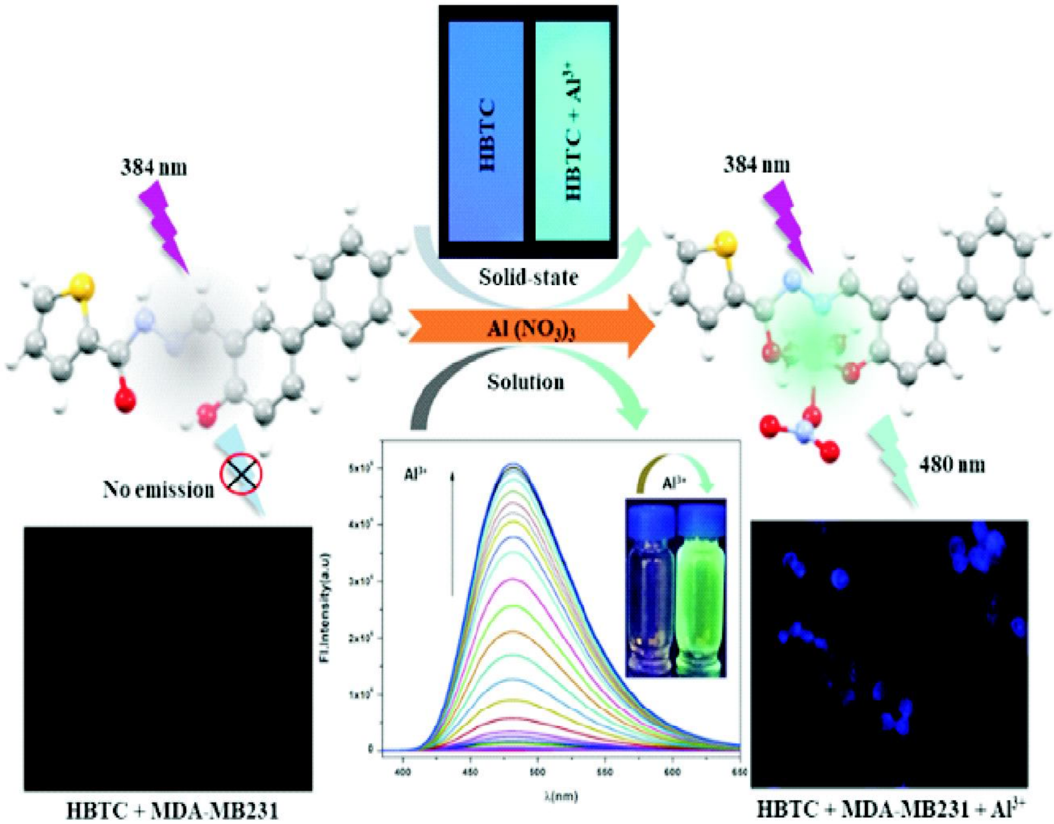
In the present work, a newly designed Schiff base chemosensor **HL**, (Z)-2,4-dibromo-6-(((piperidin-2-ylmethyl)imino)methyl)phenol constituted by condensation of 2-aminomethylpiperidine and 3,5-dibromosalicylaldehyde, has been developed to investigate its sensing efficacy towards Zn(II) and Ni(II) among various cations of comparable nature. Under UV light in methanol water (9:1) HEPES buffer it shows distinct cyan color in presence of Zn(II) and bluish cyan color in presence of Ni(II). This Zn(II)/Ni(II) recognition phenomena is further monitored by implementing UV and fluorescence study in both aqueous and semi aqueous medium. The formation of strong bond among **HL** and Ni(II)/Zn(II) is significantly characterized by the high host-guest binding constant values, obtained from electronic and fluorescence titration. As per expectation, by the reaction of **HL** and Zn(II)/Ni(II) two crystalline compounds Complex **1** and Complex **2** are formed with high luminescent property. This is due to the fact that as a consequence of crystalline compound formation, the occurrence of Chelation Enhanced Fluorescence(CHEF) introduces the moderate luminescent property in both the developed complexes. The single crystal structure revels that the asymmetric units of both the complexes comprises of two deprotonated chemosensor unit and one Zn(II)/Ni(II), forming two octahedral complexes. The calculated LOD for Ni(II) and Zn(II) sensing is in nano molar range. Complex **1** and **2** both are fluorescence active and are exposed to investigate the sensing efficacy towards ATP but interestingly Complex **2** is susceptible in recognition of ATP in full aqueous solution. Finally, the live cell imaging study confirms the bio sensing activity of the two sensors.

Contributory Paper-108

A new “turn-on” molecular switch for idiosyncratic detection of Al^{3+} ion along with its application in live cell imaging

Amitav Biswas and Tapan K. Mondal*
Department of Chemistry,
Jadavpur University,
Kolkata, West Bengal
E-mail: amitavbiswas2015@gmail.com

Among metals, aluminum is the third most abundant of all elements in the earth’s crust. It is extensively used in industrial fields such as water treatment, food additives and also in our daily life *viz*. various packing items, electrical equipment[1,2]. But excessive absorption of aluminum is harmful to human health. It sometimes leads to diseases such as Alzheimer’s disease, Parkinson’s disease, Osteoporosis and Osteomalacia[3]. Hence, it is important to develop some efficient methods for the detection of aluminum in environment. Fluorescent



sensors, owing to their simplicity, high sensitivity, instantaneous response, real-time detection and nondestructive properties, have been one of the most popular convenient methods to detect metal ions. Hence new probes for the powerful detection of Al^{3+} is highly needed. Herein we report a newly developed fluorescent probe for selective detection of Al^{3+} which involves a very simple synthetic route. The developed probe shows a sharp "turn-on" increase in emission intensity of the probe, at 480 nm upon gradual addition of Al(III) and is also effective in detection of Al^{3+} even in presence of other metal ions. The reusability and real time application of the probe were also studied. Bioimaging study reveals that the probe is also efficient to detect intracellular Al^{3+}.

References

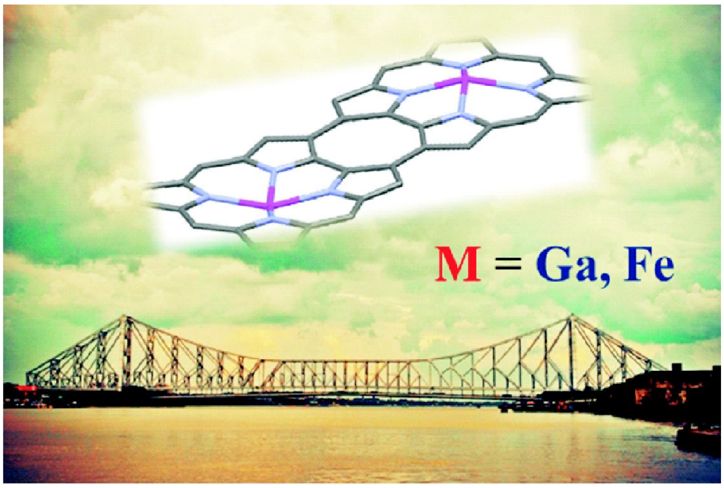
1. V. K. Gupta, M. R. Ganjiali, P. Norouzi, H. Khani, A. Nayak and S. Agarwal, *Crit. Rev. Anal. Chem.*, 2011, **41**, 282.
2. C. Lodeiro, J. L. Capelo, E. Oliveira and C. Nuñez, *Environ. Sci. Pollut. Res.*, 2016, **23**, 24419-24421.
3. L. C. Becker, I. Boyer, W. F. Bergfeld, D. V. Belsito, R. A. Hill, C. D. Klaassen, D. C. Liebler, J. G. Marks(Jr.), R. C. Shank, T. J. Slaga and P. W. Snyder, *Int. J. Toxicol.*, 2016, **35**, 16S-33S.

Contributory Paper-109

Electronic structure and electrocatalysis by fused corrole dimer

Moumita Patra[a], Tarun K. Das[b], Ujjal K. Roy[a] and Susovan Bhowmik[b]
[a]Kazi Nazrul University,
Asansol, West Bengal
[b]Bankura Sammilani College,
Bankura
E-mail: moumitaptr@gmail.com

A minor modification of the reported procedure for the synthesis of a corrole dimer $(H_3tpfc)_2COT$ that is fused by the cyclooctatetraene (COT) unit allowed for its isolation in 18% yield. The corresponding bis-gallium(III) complex was prepared as an entry into the potentially rich coordination chemistry of $(H_3tpfc)_2COT$. Both X-ray crystallography and DFT calculations disclosed that the COT moieties are essentially planar and with very unusual non-alternating and non-delocalized C-C bonds. The same holds true for the bis-gallium(III) complexes $[(Ga\text{-}tpfc)_2]COT(py)_2$ and $[(Ga\text{-}tpfc)_2]COT(py)_4$, obtained with one and two pyridine molecules coordinated to each metal ion, respectively. The electronic spectra of both the free base and the gallium(III) complexes display an extremely low energy band (λ_{max} of 720–724 nm), which points towards extensive π-delocalization through the COT bridge. Another potentially redox active metal (Fe) demonstrated efficient Proton reduction electrocatalytic activity. The poster will depict these aspects of the COT bridged corrole dimer.



References

1. *Inorg. Chem.,* 2017, **56**, 4, 2287-2296.
2. *Inorg. Chem.,* 2022, **61**, 10, 0000.

Contributory Paper-110

Impact of halogen···halogen and π-hole interactions in electrically conductivity of Cu(II)-based 1D coordination polymers

Sanobar Naaz and Mohammad Hedayetullah Mir*
Department of Chemistry,
Aliah University, New Town,
Kolkata-700 156, India
E-mail: sanobarnaaz444@gmail.com

Supramolecular chemistry has recently been explored to introduce several non-covalent interactions in the crystalline systems via the practice of crystal engineering. Although hydrogen bonding remains the utmost supramolecular force present in most chemical and biological environments, halogen bonding also share strength and directionality features similar to hydrogen bonding. Herein, two isostructural one-dimensional coordination polymers (1D CPs) $[Cu(5\text{-nip})(3\text{-Clpy})_2]_n$ (**1**) and $[Cu(5\text{-nip})(3\text{-Brpy})_2]_n$ (**2**) have been synthesized using 5-nitroisophthalic acid ($H_2$5-nip) linker and meta-substituted halopyridine, 3-chloropyridine (3-Clpy)/3-bromopyridine (3-Brpy) auxiliary ligands. The SCXRD study reveals that the CP **1** and CP **2** form 1D double chain structure with carboxylato bridged cyclic secondary building units (SBUs). Interestingly, both the CPs involve type-I halogen···halogen (X···X) interactions combined with π···π stacking interactions to generate three-dimensional (3D) supramolecular network. Moreover, both the CPs exhibit interesting X···N π-hole interactions involving nitro group as electron acceptor. Both the CPs show electrical conductivity in the semiconducting regime and behave as Schottky diodes. Interestingly, CP **1** shows higher electrical conductivity as compared to CP **2**. The higher conductivity of CP **1** is most likely related to the shorter π···π stacking of the 5-nip ligands and smaller inter-chain distance within the compound.

Reference

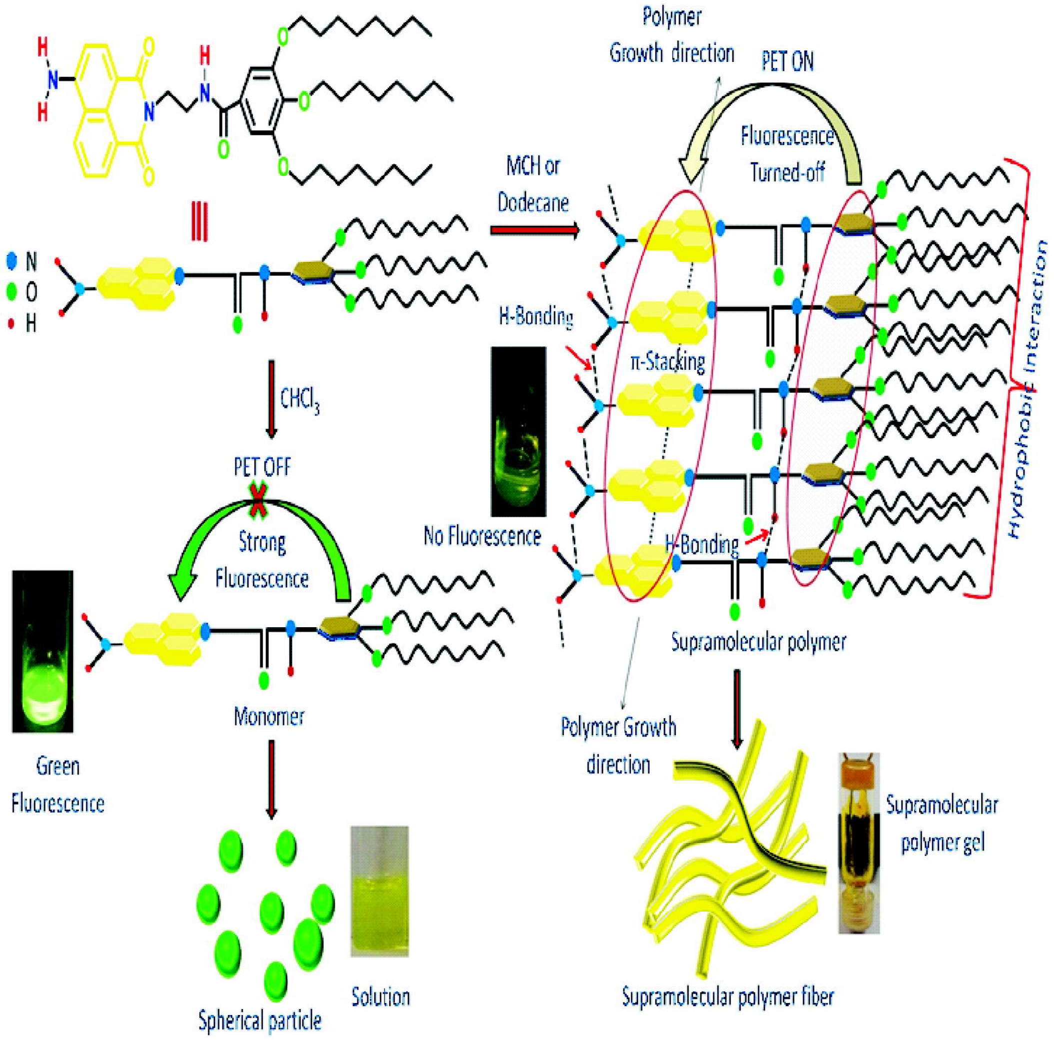
1. S. Naaz, P. Das, A. Frontera, B. Dutta, S. Khan, P. P. Ray and M. H. Mir, *Cryst. Growth Des*, Accepted for publication, 2022 (Invited article).

Contributory Paper-111

Luminescent property switching in 1D supramolecular polymerization of organic donor-π-acceptor chromophore

Sk. Mursed Ali
University of Calcutta,
Kolkata
E-mail: mursed027@gmail.com

The role of solvents in the control over supramolecular interactions has been studied for decades in protein folding, soft material fabrication and long-range organization of functional organic π chromophores. Nonpolar co-solvents (poor solvent) commonly used to initiate the supramolecular polymerization in organic solvents. It is very essential to gain more insight into the understanding of processing methodology. Hence, to investigate the influence of non-polar co-solvent composition on supramolecular polymer initiation and chain propagation, a fluorophore-spacer-receptor type naphthalimide derivative (NMI-2) has been synthesized. With the change of good solvent to poor solvent ratio, NMI-2 exhibits supramolecular polymerization in J-type fashion leading to 1D-nanowire as demonstrated by spectroscopic and microscopic studies. The efficient gel formation in non-polar solvents is evidenced by microscopic and rheological data. Analysis of co-solvent composition, temperature variable spectroscopic data and methanol experiment reveals the crucial role of a critical co-solvent composition (CCSC) to initiate the polymerization process and H-bonding followed by π-stacking interactions to propagate the polymer chain in long range order. A visual colour change due to red-shifting of intramolecular charge transfer (ICT) band and fluorescence turned-off phenomenon as a result of photo induced electron transfer (PET) from aryl receptor to naphthalimide fluorophore at the initiation of supramolecular polymerization is noted as the indicator of supramolecular polymer initiation. The observed phenomena is supported by extensive atomic force microscopic (AFM) studies and DFT calculation.



Scheme 1. Schematic representation of solvent mediated supramolecular polymerization, turned-off fluorescence and gelation.

Contributory Paper-112

Porous organic polymer for adsorptive removal of mercury: Experimental and theoretical insights

Avik Chowdhury, Sabuj Kanti Das, Saptarsi Mondal and Asim Bhaumik
Indian Association for the Cultivation of Science,
Kolkata-700 032
E-mail: chowdhury.avik28@gmail.com

The massive industrial growth due to the rapid surging of global population leads us some serious threat to mankind. Thus accumulation of industrial pollutants now a days became great concern for scientists and environmentalists. Contamination of heavy metal ions is a serious threat to human health. Mercury being originated from variety of industrial processes, oil and coal burning, mining of mercury ores, use of mercury in products and manufacturing, cement production, etc. and get contaminated on our atmosphere and aquatic resources. According to global mercury emission report given by United Nations Environment Programme (UNEP 2018), there is approximately 2000 tons of mercury emission taking place globally per year. In this work we have developed a new N-rich and sulfur-containing, secondary amine-linked, porous organic polymer TTP-1, via polycondensation of a tetrapodal amine and thiophene-2-carbaldehyde. TTP-1 displayed a high BET surface area of 1034 $m^2 g^{-1}$ with hierarchical porosity and exceptionally high uptakes of 3106 and 691 mg g^{-1} for inorganic Hg^{2+} and organic methylmercury (CH_3Hg^+), respectively. The high adsorption efficiency for mercury capture is also supported from the strong noncovalent interaction of the ligand S and N lone pairs with Hg^{2+}, as revealed from the ab initio quantum chemical calculation and AIM analysis. Cost-effective, eco-friendly and scaleable synthesis of porous organic polymer with hierarchical porosity reported herein may contribute to the design of a benchmark adsorbent for the remediation of mercury ($Hg(II)/CH_3Hg^+$) and may significantly aid in industrial and environmental cleanup.

References

1. J. O. Nriagu, *Science*, 1996, **272**, 223-224.
2. M. McNutt, *Science*, 2013, **341**, 1430.
3. D. P. Krabbenhoft and E. M. Sunderland, *Science*, 2013, **341**, 1457-1458.
4. Global Mercury Assessment 2018, UNEP, UN Environment, 2019.

Contributory Paper-113

Effect of end-on/end-to-end azide bridging of versatile dimeric/polymeric Cu(II) complexes in bio-relavent catalytic activity, DNA/Protein binding efficacy and anticancer activity studies: Combine experimental and theoretical approach

Biman Ari and Tithi Maity*
Prabhat Kumar College, Contai,
Contai-72404, Purbamedinipur, West Bengal, India
E-mail: bimanari@gmail.com

Two new versatile azide bridged Cu(II) complexes, $[Cu(L_1)(\mu_{1,1}\text{-}N_3)(DMF)]_2$ (**1**) and $[Cu(L_2)(\mu_{1,3}\text{-}N_3)]_\alpha$ (**2**) have been synthesized using two different N_2O donor Schiff bases namely (Z)-4-bromo-2-(((piperidine-2-ylmethyl)imino)methyl)phenol (**HL_1**) and (E)-4-chloro-2-(((2-(-1-yl)imino)methyl)phenol(**HL_2**) respectively. The single crystal X-ray diffraction analyses reveal that complex **1** is an end-on azido-bridged dinuclear Cu(II) complex whereas complex **2** consists of end-to-end azido-bridged polymeric network. The formation of such 1D polymeric structure of complex **2** is further rationalised with theoretical calculations. After routine characterization both the complexes are exploited as model enzyme to check their catecholase- like activity in DMF medium where complex **1** turns out to be more competent in comparison with **2**. The biomedical applicability of these two complexes are evaluated via determining their thorough interaction with DNA and HSA adopting several spectroscopic approaches. The electronic absorption spectra indicate remarkably high binding constant values for both the complexes with DNA and HSA (order ~ 10^5). Interestingly complex **1** and **2** show different binding mode with DNA as revealed from various experimental observations like fluorescence quenching, CD and viscosity measurements etc. The theoretical approach by means of molecular docking study successfully explained the fact depending upon the structural diversity of the complexes. In continuation the cytotoxic effect of both the complexes are studied on HeLa (cervical cancer cell), PA1 (ovarian cancer cell) and wi32 fibroblast (normal cell) cell line via does and time dependent manner. The LD_{50} values clearly display high anticancer property of complex **2** than **1** which can further be correlated with its higher DNA and HSA binding ability. Finally the AO/PI staining technique was adopted to visualize the nuclear morphological changes of cancer cell (HeLa) after treatment with complex **1** and **2** and also to determine the cell death mechanism.

Contributory Paper-114

An efficient approach for the synthesis of Novel 8-substituted-2,5-dihydro-2-(2-nitrophenyl)-4-(2-thienyl)-1,5-benzothiazepines

Madhuri Kandalkar* and Priyanka Sharma
School of Engineering & Sciences,
GD Goenka University,
Gurugram, Haryana
E-mail: madhuri.keote@gmail.com

Various methods of synthesis of heterocycles benzothiazepine moiety has been resulted in the construction of variety of innovative and interesting reactions. The biologically active shield structure of 1,5-benzothiazepines has been reported to be of immense chemotherapeutic applications. The flexibility in the methods of synthesis of this scaffolding has prompted the researchers to search improved synthetic routes for synthesis of series of novel bicyclic benzothiazepines over the conventional methods. The present study is focused to explore an efficient syntheses of α,β-unsaturated carbonyl system in different reaction conditions and their reactions with 5-substituted-2-aminothiophenols, substituents being halogens and alkyl to get a series of novel 8-substituted-2,5-dihydro-2-(2-nitrophenyl)-4-(2-thienyl)-1,5-benzothiazepine derivatives by mere 20 minutes swirling in diethyl ether at room temperature. This synthetic approach provides shorter reaction time, mild reaction conditions and good yield. The structural characterization have been accomplished by micro estimations for C, H, N and ^{1}H NMR.

Contributory Paper-115

Phenothiazine-napthalene based photosensitizer: An Ideal choice for acne removal therapy

Shrabani Barman
Krishnath College,
Berhampore, Murshidabad, West Bengal
E-mail: shrabanibarman@gmail.com

Photodynamic therapy (PDT) is a new emerging therapy, clinically proved, minimally invasive therapeutic procedure, has been added a new flavour in dermatology. Use of light absorbing chromophore (absorb light 400–600 nm) make PDT a further ahead choice only by increasing the light absorbing ability to the target cells in the surface of the skin. Phenothiazine – napthalene based photosensitizer, a best choice because of its yellow light absorbing ability, which is transparent to the skin.

Contributory Paper-116

Use of an amphiphilic block copolymer synthesized by atom transfer radical polymerization technique in stabilizing gold nanoparticles

Suparna Guha
Department of Chemistry,
Bhairab Ganguly College, Belgharia,
Kolkata-700 056
E-mail: sguhasanak@gmail.com

Metal nanoparticles have wide applications due to their characteristic physical and chemical properties which are quite different from the macroscopic regime. They exhibit unique size dependent electrical, magnetic and optical properties. Generally metal nanoparticles are produced by the reduction of a metal salt using a suitable reducing agent either in aqueous or organic medium in micelle or reverse micelle forms. Various surfactants, citrates and also polymers are commonly used as stabilizing agents. The use of polymers as stabilizing agents has some virtues i.e. (a) a small concentration of homo or block copolymer is required (b) a functionalized polymer can act both as a stabilizing as well as a reducing agent (c) the ease of preparation of metal – polymer nanocomposites.

In this work we have synthesized a block copolymer polymethylmethacrylate-b-poly[2-(N,N-dimethylamino)ethylmethacrylate] by atom transfer radical polymerization technique. The polymer had a narrow polydispersity index. This block copolymer is amphiphilic in nature having a hydrophilic poly 2-(N,N-dimethylamino)ethylmethacrylate end and a hydrophobic polymethylmethacrylate end. The block copolymer was then used to stabilize gold nanoparticles in aqueous as well as in water-tetrahydrofuran medium at room temperature. The block copolymer acted both as reducing agent and stabilizing agent. The nanoparticles were characterized by taking Transmission Electron Microscope images and Dynamic Light Scattering experiments. The absorption spectra were also taken by a UV-visible Spectrophotometer.

Contributory Paper-117

A novel covalent organic framework as a metal free electrocatalyst for efficient hydrogen evolution reaction

Santu Ruidas
Indian Association for the Cultivation of Science,
Kolkata-700 032
E-mail: santuruidas803@gmail.com

We have developed a metal free triazine based covalent organic framework via solvothermal Schiff base condensation reaction by reacting two monomers 2-hydroxybenzene-1,3,5-tricarbaldehyde and 4,4′,4″-(1,3,5-triazine-2,4,6-triyl)tris([1,1′-biphenyl]-4-amine). This COF offers high surface area of 928 m^2/g with crystallinity and has displayed excellent HER activity in the electrochemical water-splitting with a very low overpotential of 200 mV and specific activity of 0.2831 mA/cm^2 together with high retention in the catalytic activity after a longer duration of electrocatalysis in aqueous solution of 0.5 M H_2SO_4. The DFT calculations suggest that the electron deficient carbon sites near the π electron-donating nitrogen atoms are more active towards HER than carbon sites near the electron-withdrawing nitrogen and oxygen atoms.

Contributory Paper-118

Synthesis, characterization and biological activity studies of mononuclear Copper(II) complexes derives from azo containing novel *O,O* donor ligands

Avijit Sarkar
Department of Chemistry,
Bhairab Ganguly College,
Kolkata-700 056, India
E-mail: rite2avijit@gmail.com

Azo linked salicyldehyde and a new 2-hydroxy acetophenone based ligands (HL1 and HL2) with their copper(II) complexes $[Cu(L1)_2]$ (**1**) and [Cu(L2)2] (**2**) were synthesized and characterized by spectroscopic methods such as ^1H, ^{13}C 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 $6.5\pm$ 0.3×10^3 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

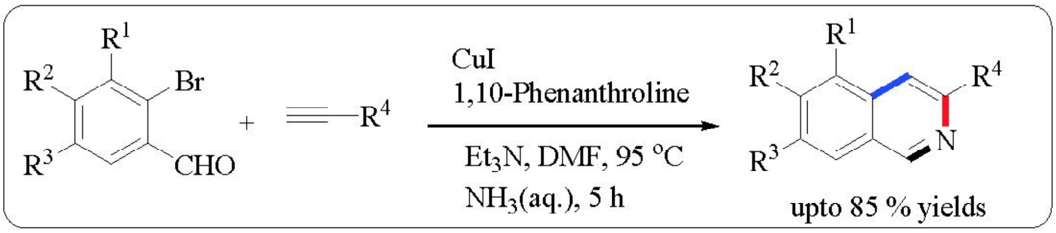
1. Synthesis, characterization and nucleic acid binding studies of mononuclear copper(II) complexes derived from azo containing *O*, *O* donor ligands" NUCLEOSIDES, NUCLEOTIDES AND NUCLEIC ACIDS, 20018, **37**, 10, 563-584.

Contributory Paper-119

Synthesis of isoquinoline using Cu-mediated one-pot tandem cross-coupling and cyclization

Shubhendu Dhara
Department of Chemistry,
Bhairab Ganguly College,
West Bengal State University,
Kolkata-700 056
E-mail: dharashubhendu@gmail.com

Phenanathridines and its higher analogs benzophenanthridines are prevalent in naturally occurring compounds of potent chemical and bio-activity. One-pot synthetic strategy has been developed to access isoquinolines and its analogs *via* Cu-mediated tandem cross-coupling and cyclization in good yields under mild reaction conditions. A mixture of suitably substituted a-bromoaldehyde, terminal alkyne, and aq NH_3 in CuI/1,10-phenanathroline catalytic system afforded the 3-substituted isoquinoline regio-selectively in good to excellent yields. This methodology is a very general one with the tolerability to a range of substituent and synthetically useful yield of products. This one step procedure would have bene fit the total synthesis of complex natural and unnatural compounds of important biological potential.



Scheme. Synthesis of isoquinoline.

References

1. M. Croisy-Delcey, A. Croisy, D. Carrez, C. Huel, A. Chiaroni, P. Ducrot, E. Bisagni, L. Jin and G. Leclercq, Diphenyl quinolines and isoquinolines: Synthesis and primary biological evaluation. *Bioorg. Med. Chem.*, 2000, **8**, 2629.
2. C. Si and A. G. Myers, A versatile synthesis of substituted isoquinolines. *Angew. Chem. Int. Ed.*, 2011, **50**, 10409-10413.
3. A. H. Zhang, N. Jiang, W. Gu, J. Ma, Y. R. Wang, Y. C. Song and R. X. Tan, Characterization, synthesis and self-aggregation of (-)-Alternarlactam: A new fungal cytotoxin with cyclopentenone and isoquinolinone scaffolds. *Chem.–Eur. J.*, 2010, **16**, 14479.

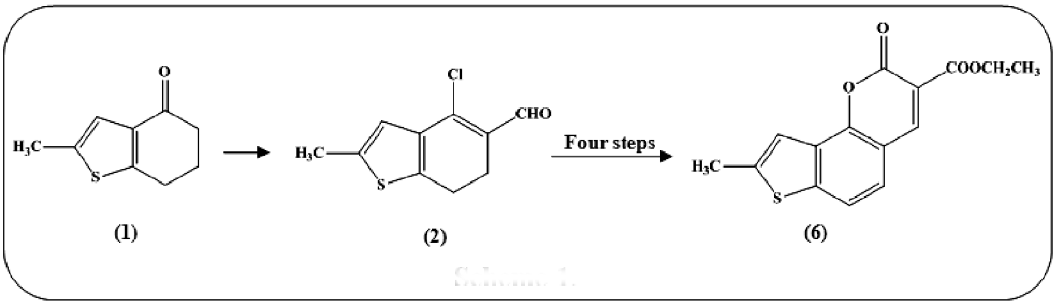
Contributory Paper-120

Solvent effect and metal ion sensing by synthesized novel thiophene analogue of angelicin derivative using fluorescence study

Tuyan Biswas, Arnab Halder and Gandhi Kumar Kar
Department of Chemistry,
Presidency University,
Kolkata-700-073
E-mail: biswastuyan@gmail.com
arnab.chem@presiuniv.ac.in
gandhi.chem@presiuniv.ac.in

Angelicin, naturally occurring photoactive furocoumarin derivatives, are a very promising compound for therapeutic study[1]. Our aim is to design and synthesis of novel thiophene analogues of angelicin derivative and its photoluminescence property. Starting from 2-methyl-6,7-dihydrobenzo[b]thiophene-4(5H)-one (**1**) the synthesis is involved five steps, where Vilsmeier Haack reaction was the first step followed by addition-elimination by methoxide ion, condensation with cyanoacetic ester, cyclization and aromatization (Scheme 1). The synthesized compounds are characterized by ^{1}H NMR, ^{13}C NMR and HRMS.

We have estimated experimentally the ground and excited state dipole moments of synthesized angelicin derivative ethyl 8-methyl-2-oxo-2H-thieno[2,3-h]chromene-3-carboxylate (**6**) by the solvatochromic shift method based on the spectral shift of absorption and fluorescence maximum. Quenching of photoluminescence for the concerned moleculeis performed to understand its mode of interaction with quencher and for the sensing of environmentally and biologically relevant metal ions. It shows “Off-Sensing” fluorescence selectivity toward Fe^{3+} and Fe^{2+} ions at neutral pH range over other metal ions. The Stern-Volmer plot shows non-linearity with upward curving but the modified Stern-Volmer plot for



Scheme. 1

both Fe^{3+} and Fe^{2+} is linear and the quenching constant are calculated $K_{[Fe3+]} = 7.48 \times 10^2$ M^{-1} and $K_{[Fe2+]} = 9.01 \times 10^2$ M^{-1} respectively.

Reference

1. C. K. Mahendra, L. T. H. Tan, W. L. Lee, W. H. Yap, P. Pusparajah, L. E. Low, S. Y. Tang, K. G. Chan, L. H. Lee and B. H. Goh, Angelicin- A furocoumarin compound with vast biological potential, *Frontiers in Pharmacology*, 2020, **11**, 366. [related references are cited therein].

Contributory Paper-121

Adsorptive removal of crystal violet from its aqueous solution using coconut coir and its acid-treated forms

Tamasha Chatterjee, Indrajit Ghosh, Sayanti Kar and Sudip Kumar Das
Chemical Engineering Department,
University of Calcutta,
92, Acharaya Prafulla Chandra Road,
Kolkata-700 009
E-mail: tamasha1995@gmail.com
drsudipkdas@gmail.com

Water pollution has turned into a significant environmental problem. Pollution of natural water bodies due to the release of dye-containing wastewaters from textile, cosmetics, food colouring and paper industries becomes a genuine issue. Crystal violet (CV) is used in dyeing textiles and paper colouring industries. CV is a mutagen and mitotic poison, and it can form a protein-dye complex and hence acts as an enhancer for bloody fingerprints. CV is carcinogenic and has been classified as a calcitrant molecule; since microorganisms poorly metabolize it, it can persist in various environments. This research aims to carry out a batch study to remove toxic crystal violet by natural adsorbent coconut coir and its acid-treated forms. The adsorbents are natural coconut coir (UCC), phosphoric acid-treated coconut coir (PCC) and sulphuric acid-treated coconut coir (SCC). The adsorbent characterizations were established through SEM, XRD, FTIR and BET. The batch experiments for crystal violet removal were carried out with the change of process variables, i.e., pH, adsorbent dose and contact time. At optimum process conditions, the maximum crystal violet removal was 90.78% for PCC. Different well-known kinetic models were tested with the experimental results, showing that the pseudo-second order kinetics is fitted best. The isotherm study shows that the Langmuir model (r2) is better; hence, the process principally involves monolayer adsorptions. The sorption energy calculated using the D-R isotherm showed the physical adsorption process. The thermodynamic study indicated that the adsorption process was exothermic. This research suggests that coconut coir and its acid-treated forms suit crystal violet removal from wastewater.

Contributory Paper-122

Validation of molecular docking tools by screening of MAO-A inhibitor as anti-depressant

Abhimannu Shome and Pooja A. Chawla
Department of Pharmaceutical Chemistry,
ISF College of Pharmacy, Moga,
Moga
E-mail: abhimannu007shome@gmail.com

Long-term effects of quarantine during the COVID-19 epidemic included several mental health problems such as depression, anxiety, rage and post-traumatic stress disorder. According to world health organization report, depression increased by a massive figure of 25% in world wide during and post-Covid time Monoamine oxidase (MAO-A), a mitochondrial enzyme, is a common target in the development of antidepressant drugs. Neurotransmitters including serotonin, dopamine and norepinephrine are critically degraded by MAO, which lowers their levels and frequently causes depression. For this investigation, pre-reported 23 substances with established IC50 values were chosen from different articles. Following the screening, MAO-A and MAO-B inhibitors based on pyrazolines were gathered and docking was carried out in Glide using the MM-GBSA force field. This led to a number of substantial docking scores with encouraging RMSD. The PLANT method, which consists of the ant colony optimization-based PLANTPLP and the empirical scoring function PLANTCHEMPLE, was employed by another docking service. In the rating of the study's accuracy, PLANT>Glide was proposed by the G correlation in the validation of two molecular docking tools. Although PLANT had a promising correlation with very little outlier, this analysis revealed that the correlation model of Glide looked to be statistically less correlated.

Contributory Paper-123

Biphenyl containing amido Schiff base derivative as a turn-on fluorescent chemosensor

Anamika Hoque and Md. Akhtarul Alam*
Department of Chemistry,
Aliah University, New Town,
Kolkata-700 156, India
E-mail: anamikahoque35@gmail.com

A hydrazine derived Bis(2-hydroxybenzylidene)-[1,1′-biphenyl]-2,2′-dicarbohydrazidehas been synthesized and its sensing properties towards metal ions has been demonstrated using simple UV-visble spectroscopic, fluorometric technique and visible colour change. The compund shows high fluorescence selectivity and sensitivity towards Al^{3+} and Zn^{2+} ions in aqueous DMF media. The fluorescent intensity of this increases in the presence of Al^{3+} at 458 nm and in presence of Zn^{2+} at 478 nm. Visual colour change under 350 nm UV light, exhibit a bluish-white and bluish-yellow fluorescence light in presence of Al^{3+} and Zn^{2+} ion respectively. The ESI-MS and the Job's plot analysis shows that the compound and metal ions formed 1:2 coordination complex. Fluorescence switch based on the control of Zn^{2+} and EDTA proved that the compound could act as reversible chemosensor. However, on addition of EDTA into Al^{3+} complex, there was no spectral change as well as naked-eye colour change was observed. The sensing behavior was also studied with molecular logic function of AND gate. Furthermore, "Test Kits" coated with compound showed a successful selective detection of Al^{3+} ion under UV light.

Reference

1. Anamika Hoque, Md. Sanaul Islam, Mehebub Ali Khan, Soumen Ghosh, Md. Asraful Sekh, Sahid Hussain and Md. Akhtarul Alam, *New J. Chem.*, Accepted for publication, 2022.

Contributory Paper-124

A novel semiconducting Zn-based metal thiolate framework as a potential photoanode in photoelectrochemical water oxidation reaction

Anirban Ghosh
Indian Association for the Cultivation of Science,
Jadavpur,
Kolkata, West Bengal
E-mail: anirbanju1995@gmail.com

Designing an efficient photocatalyst for sustainable photoelectrochemical (PEC) water oxidation reaction is always a quest to researchers in the context of green energy research. Here, we have introduced a novel semiconducting Zn-MOF which we coined as metal thiolate framework through successful stitching of an “N” donor linker with a triazine-based tristhiolate secondary building unit in the overall architecture. The incorporation of both linker and tristhiolate ligand synergistically modulate the architecture as rigid, crystalline, three-dimensional, thermally stable and porous. This new zinc thiolate framework is performed as an n-type semiconductor as evidenced from UV-Vis DRS spectroscopy, AC and DC conductivity analysis and Mott-Schottky diagram. Now this n-type semiconductor material is utilized as a suitable nontoxic, cost effective photoanode in PEC water oxidation due to its high efficiency for solar light driven oxygen evolution reaction in KOH medium using standard Ag/AgCl as the reference electrode. The superiority of this material was further revealed from the low onset potential (0.822 mV vs RHE), high photocurrent density (0.204 mA/cm^2), a relevant durability, high O_2 evolution rate (77 μmol g^{-1} of oxygen evolution within 2 h) and a good efficiency (ABPE 0.42%, IPCE 29.6% and APCE 34.5%). Further, porosity in the overall framework helps the PEC performance due to better mass diffusion of the electrolyte. A detailed mechanism for the OER reaction was analyzed through DFT analysis suggesting potential future of this Zn-thiolate framework for achieving high efficiency in sustainable water oxidation reaction.

Contributory Paper-125

Extraction of phyto bioactive compounds using green solvents and environment friendly sustainable extraction techniques

Debashree Debasish Das and Pooja A. Chawla
Department of Pharmaceutical Analysis,
ISF College of Pharmacy, Moga,
Moga
E-mail: dasdebashreedebasish1998@gmail.com

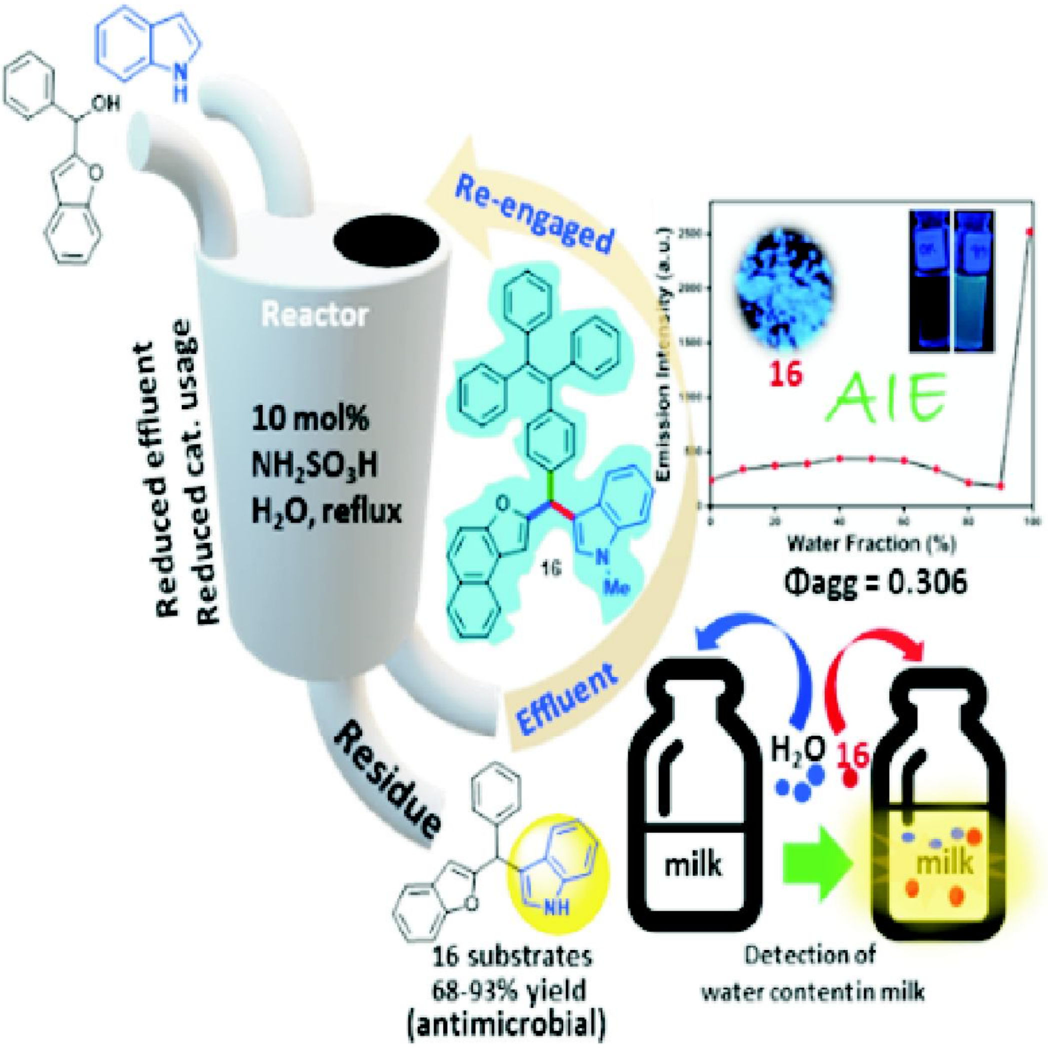
The extraction of compounds using novel extraction technologies and green solvents through nontoxic extraction routes have been widely used in different food industries to minimize degradation and enhance extraction yields in response to consumer demand for greener alternatives to toxic chemical products as well as sustainable industrial concerns. Green technologies are now regarded as a contemporary industrial process. Studies have shown that these cutting-edge extraction techniques, such as microwave-assisted extraction (MAE), ultrasound-assisted extraction (UAE), microwave-assisted extraction (MAE), and their combinations, such as ultrasonic microwave-assisted extraction (UMAE), ultrasound-assisted enzymatic extraction (UAEE), microwave-assisted enzymatic extraction (MAEE), etc., exhibit greener, cleaner, and higher potential extraction abilities, but in some cases we use specific equipment. The use of more environmental friendly and more potential solvents such as supercritical fluids, deep eutectic solvents and ionic liquids occurs since they constitute the basis of the extraction process. When selecting an appropriate extraction technique and solvent, it is important to strike a balance between the product's quality and price as well as the process' efficiency. The solvent should also be environmentally benign. Here, we cover revolutionary green solvent technology and sustainable novel extraction methods employed in the extraction of phytobioactive chemicals, as well as their mechanism, influencing factors, process, advantages and limitations.

Contributory Paper-126

On-water dehydrative substitution reaction to access unsymmetrically substituted triarylmethanes (TRAM's) and developing TRAM based AIEgen

Gauravi Yashwantrao, Prapti Shetty, Parimal J. Maleikal,
Purav Badani and Satyajit Saha*
Department of Speciality Chemical Technology,
Institute of Chemical Technology, Mumbai,
Mumbai-400019, Maharashtra
E-mail: yashwantraogauravi1895@gmail.com
ss.saha@ictmumbai.edu.in

Employing water as a reaction media in chemical transformation has several advantages in terms of safety, non-toxicity, cost and abundance. However, a dehydrative substitution reaction in an aqueous medium is a highly challenging operation. Here, we have reported a sulfamic acid-mediated dehydrative substitution reaction of benzofuryl alcohols with several nucleophiles in water towards the scalable synthesis of unsymmetrically substituted TRAMs in good to excellent yields. The ability to achieve dehydration in water to access the triarylmethanes in high yields with the ability to re-engage the aqueous effluent for subsequent batch operations undoubtedly has reduced the environmental burden by minimizing the effluent discharge as well as catalyst usages and simplified the product recovery by filtration. Moreover, we have realized that when aptly designed, these propellor-shaped triarylmethanes can become an ideal candidate to promote aggregation-induced emission (AIE) through restricted intramolecular rotation. Therefore, the methodology was further extended towards developing a green synthetic route to access triarylmethane based solid-state emitting materials with irreversible mechanoflurochromic property which was engaged to monitor the added water content in the milk sample.


OH
O
N
H
Reactor
10 mol%
NH_2SO_3H
H_2O, reflux
Reduced effluent
Reduced cat. usage
Re-engaged
O
16
N
Me
Emission Intensity (a.u.)
2500
2000
1500
1000
500
0
0
20
40
60
80
100
Water Fraction (%)
16
AIE
Φagg = 0.306
Effluent
Residue
H_2O
16
milk
milk
O
NH
16 substrates
68-93% yield
(antimicrobial)
Detection of
water content in milk

Contributory Paper-127

Microwave assisted synthesis is an environmental benign green chemistry approach: Fact or myth?

Keshav Taruneshwar Jha* and Pooja A. Chawla
Department of Pharmaceutical Chemistry,
ISF College of Pharmacy, Moga,
Moga
E-mail: keshavlion1998@gmail.com

Microwave assisted synthesis showed a revolution in the chapter of green chemistry. In chemistry laboratory MAS helped to carry out many transformations with greater efficiency. The green chemistry is the exercise of designing the process which reduces the use as well harmful material production. Microwave assisted synthesis offers most efficient, reliable and fast synthesis of certain organic compounds and these reactions play an enormous role in organic synthesis. The green chemistry has 12 principles which are correlated to each other which generally states about the prevention of waste, design of energy efficient process and the use of new analytical procedures. Microwave synthesis is contemplated as lead approach in green chemistry because it is environment friendly and has potentially greater impact in organic synthesis. MAS possess faster reaction, high purity, energy saving and hence it is environment benign compared to other conventional methods. Certain organic reactions have been carried out using MAS with conventional methods.

Contributory Paper-128

Development of some simple feasible chemosensors for the detection of Zn(II) with formation of solid crystalline compound and their versatile Bio-applications

Manik Das and Tithi Maity*
Department of Chemistry,
Prabhat Kumar College, Contai,
Purbamedinipur-721 404, West Bengal, India
E-mail: manikdas12012@gmail.com

Several Schiff base Chemosensors **H_3L1**(6,6′-((1E,1′E)-((2-hydroxypropane-1,3-diyl)bis(azaneylylidene))bis(methaneylylidene))bis(2-ethoxyphenol) – **[A]**, **HL2** ((E)-4-Chloro-2-(((2-(perazine-1-yl)ethyl)imino)methyl)phenol– **[B]**, **HL3** (4-chloro-(((2-(piperidine-1-yl)imino)methyl)phenol) – **[C]** and **HL4** ((E)-2-(((4-bromophenyl)imino)methyl)phenol **[D]** have been fabricated by one step simple condensation of 1, 3 diamino 2-propanol with 3-ethoxy salicylaldehyde, 2-aminoethyl Pierazine with 5-Chlorosalicylaldehyde, 2-aminoethyl piperidine with 5-Chlorosalicylaldehyde and 4-Bromo aniline with 5-Bromosalicylaldehyde respectively for easy and selective reorganization of Zn(II) ion through formation of crystalline solid complex in aqueous and semi aqueous media. The optically monitored sensing phenomena has been further assessed by implementing UV-vis Spectroscopy, Fluorescence Spectroscopy. LOD for Zn(II) was determined in the range of 10^{-7}(*M*). High probe-analyte binding constant values indicate the strong host-guest binding which can be validated by the formation of crystal with impressive luminescence property. NMR, MASS Spectral data, Density Functional Theory (DFT) and single crystal data analysis unveils the host–guest binding mechanism. The *in vitro* cell imaging study gives an authentic hints for *in vivo* biomedical application of the ligands as a selective and easy Zn(II) sensor. The luminescence property of Zn(II)-**C** complex is further used for specific detection of Al(III) in aqueous media whereas Zn(II)-**D** complex is further exposed to investigate its DNA and HSA binding efficacy. The macromolecular interaction as well as sensing property of metalloligandis spectroscopically assessed.

Contributory Paper-129

Degradation of polycyclic aromatic hydrocarbons in soil: An effect of an eco friendly oxidizing agent, Fenton Reagent

Mizanur Rahman* and Prahash Chandra Sarma
*Department of Chemistry, Hatsingimari College,
Hatsingimari, Assam
Department of Chemistry, Cotton University,
Guwahati, Assam, India
E-mail: mizan99542@gmail.com

The carcinogenicity and bioavailability of a few Polycyclic Aromatic Hydrocarbons (PAH) has become a matter of serious concern due to their Long exposure on soil. Soil is the receptor of large number of aromatic hydrocarbons where from the bioavailable ones enter the living kingdom and continue its bioaccumulation and bio magnifications. It starts its detrimental effects as soon as it crosses the permissible level. Since PAH are of recalcitrant nature and hydrophobic, there is the chance of adsorption of these on soil, sediments etc. in water bodies. As such soil and sediments in river bed are prone to be a storehouse of persistent PAH in areas where river water carries effluents especially from refineries, oilfields, coal fields etc. The biodegradation process is a process of oxidation. In the present experiment, the influence of an eco friendly oxidizing agent Fenton's Reagent (FR) on a mixture of four PAH viz. Anthracene(ANT), Fluorene(FLN), Naphthalene(NPH) and Phenanthrene(PHN) placed in river bed soil is examined in a 60 days experiment. The experimental soil samples are taken from river bed of the river Brahmaputra in the district of Dhubri, Assam, India. A few important physico-chemical parameters of the soil were monitored before placement of measured quantity of PAH. pH is measured at every 20 days of the experimental period.

It has been found that the texture of the experimental soil is Loamy sand; deficient of organic carbon compared to agricultural soil and possesses slightly alkaline soil reaction. Gravimetric determination of the soxhlet extracts shows that the extent of degradation in samples where FR was applied in the reagent ratio of $H_2O_2 : FeSO_4 = 10:1$ is more compared to samples without applied FR. From the GC chromatograms, it has been seen that the mechanism of degradation in presence of FR is quite different from without FR. In a 34 minutes GC analysis, where 50 prominent peaks were recorded in the chromatograms; the samples with FR has only 12, 7 and 7 common peaks with the sample without FR in the soxhlet extracts of 0, 20 and 40 days respectively. On the other hand, the number of common peaks in the samples without FR is more compared to number of common peaks in samples with FR indicating lower rate of degradation in absence of FR. It has been assumed that concentration of ferrous ions in the 10:1 reagent ratio is not high enough to scavenge hydroxyl radicals which would reduce degradation efficiency of FR.

Contributory Paper-130

Advanced green analytical techniques for food analysis

Nikita Sharma* and Pooja A. Chawla
Department of Pharmaceutical Analysis,
ISF College of Pharmacy, Moga,
Moga
E-mail: niki94353@gmail.com

Analytical methods and techniques have been developed and used in the field of food science in response to the increased concern people have over what is in their food and its safety. The detrimental effects of food toxicants and pesticide residues provide complicated obstacles for food analysts, which are thereby reduced by a number of cutting-edge technologies. The development of greener analytical techniques is a topic of great interest. Green analytical chemistry seeks to minimise or completely avoid the use of hazardous materials, the generation of waste and the use of *in situ* and *in vivo* technologies in place of screening techniques for simple qualitative tests. Conventional analytical methods can be used to determine the quality of food, but they are time-consuming, labor-intensive, and frequently lead to environmental contamination (toxic wastes). They also call for toxic and non-biodegradable organic solvents, which are inconsistent with the principles of green chemistry. Recent developments in analytical methods is time efficient, environmentally friendly, which is based on nanobiotechnology and ultrasensitive detection of food and environmental samples. Hybrid techniques used in this study include Gas Chromatography-Mass Spectrometry (GC-MS), Liquid Chromatography-Mass Spectrometry (LC-MS), High Resolution Mass Spectrometry (HRMS) and some modern extraction techniques like Magnetic Solid Phase Extraction (MSPE), Enzymatic immunoassay (ELISA), which is frequently used to extract food and pesticides.

Contributory Paper-131

Graphene-bentonite supported free-standing, flexible membrane with switchable wettability for selective oil-water separation

Pratik S. Dhumal, Rahul V. Khose, Pravin H. Wadekar,
Kshama D. Lokhande and Surajit Some*
Department of Speciality of Chemicals Technology,
Institute of Chemical Technology, Mumbai,
Maharashtra-400 019
E-mail: sr.some@ictmumbai.edu.in

In this research, we have prepared, flexible, sodium-bentonite-fabricated graphene (SBG) composite membrane for oil water separation. Simple vacuum filtration and coating techniques were used to prepare the membrane and it was successfully applicable on filter paper and cotton cloth which are used as membrane for oil water separation. With the selective application of water, oil, or an organic solvent, the SBG composite membrane's switchable wettability capabilities allowed it to change the surface's separation from hydrophilic/oleophilic to hydrophobic/oleophilic. The as-prepared membrane has high efficiency (>98%) to separate oil-water mixtures, good recyclability (96% efficiency after 10 cycles), a high flux of 625 Lm^{-2} h^{-1} and a good oil rejection ratio (>97%). The SBG composite can easily be scaled to separate the oil-water mixture for industrial applications. Furthermore, the advantages of the membrane are its easy preparation, self-cleaning property, switchable wettability property (hydrophilic/oleophobic to hydrophobic/oleophilic and vice versa), high flux and excellent recyclability for the selective separation of oil/organic solvents and water from their mixtures.

Contributory Paper-132

Construction of near-infrared fluorescent dual targeting mechanically interlocked molecules for live cancer cell specific lysosomal staining and multicolor cellular imaging

Rabi Sankar Das and Samit Guha*
Department of Chemistry,
Organic Chemistry Section,
Jadavpur University, India
E-mail: samitfsu@gmail.com
samit.guha@jadavpuruniversity.in

Herein, we have designed bright near-infrared (NIR) fluorescent mechanically interlocked molecules with dual targeting functionality. Two RGDS peptides are conjugated at the macrocycle and a morpholine moiety is tethered at the axle for live cancer cell specific active targeting followed by selective internalization in malignant lysosomes. We have used click chemistry using copper(I)-catalyzed azide-alkyne cycloaddition on the Wang resin to synthesize NIR rotaxane/RGDS conjugates. This solid phase click chemistry on the Wang resin allows easy purification with descent yield of rotaxane/RGDS conjugates. Live cancer cell selective malignant lysosome targeting and NIR imaging using rotaxane [LysoSQRot-(RGDS)$_2$] is demonstrated and compared with control rotaxane molecules using confocal laser scanning microscopy. Moreover, LysoSQRot-(RGDS)$_2$ probe in combination with other organelle specificic dyes with distinct excitation and emission have been used in multicolor imaging of live HeLa cells. Single crystal X-ray structures confirm the formation of macrocycle, unsymmetrical squaraine axle and rotaxane molecules. LysoSQRot-(RGDS)$_2$ is a highly attractive probe due to its water solubility, active targeting of live cancer cells followed by selective internalization in malignant lysosomes, high stability towards biological nucleophilic attack, photostability, intense and narrow NIR absorption/emission bands with multicolor imaging application and high quantum yield.

References

1. C. Zhai, C. L. Schreiber, S. P. Coley, A. G. Oliver and B. D. Smith, *Angew. Chem. Int. Ed.,* 2020, **59**, 23740-23747.
2. R. S. Das, P. C. Saha, N. Sepay, A. Mukherjee, S. Chatterjee and S. Guha, *Org. Lett.,* 2020, **22**, 5839-5843.

Contributory Paper-133

Adsorptive elimination of methylene blue dye from aqueous solution by chitosan-*n*SiO_2 nanocomposite - isotherm, kinetic, thermodynamic, desorption study and scale-up design

Samanwita Bhattacharya, Baisali Rajbansi and Sudip Kumar Das
Department of Chemical Engineering,
University of Calcutta,
92, Acharaya Prafulla Chandra Road,
Kolkata-700 009, India
E-mail: samanwita_bhattacharya@yahoo.co.in
drsudipkdas@gmail.com

Heavy metals and organic dyes in water in concentrations exceeding the tolerable limit are unsafe for aquatic life and humans. Chitosan nanocomposites show a potential adsorption capacity to organic dyes. The present study encompasses the preparation of chitosan-*n*SiO_2 nanocomposites (CSNC) with different weight ratios of chitosan to *n*SiO_2 and its application in the methylene blue (MB) dye adsorption. The nanocomposites are characterized with the help of SEM, BET, FTIR, XRD and TGA. The adsorption experiment is performed in batch mode under varying experimental conditions. Several isotherm and kinetic models are analyzed with the experimental data and thermodynamic conditions required for adsorption are also determined. Maximum Langmuir adsorption capacities of the adsorbents for MB varied in the range 21.32-31.34 $mg.g^{-1}$. The pseudo-second order model is the best-fitted kinetic model concerning all three adsorbents. Safe disposal of the used adsorbents, the desorption study and scale-up design are also carried out.

Contributory Paper-134

Towards "Safer & Better Batteries"-Engineered solid state electrolyte derived from biowaste for next generation solid state lithium batteries: Focus on impeding lithium dendritic migration path

Kuntal Ghosh and Mir Wasim Raja
Energy Materials and Devices Division (EMDD),
CSIR-Central Glass & Ceramic Research Institute,
196, Raja S. C. Mullick Road,
Kolkata-700 032, West Bengal, India
E-mail: kuntalghosh1004@gmail.com

Need for Better battery (Energy density & Safety)

Afterfirst successful commercialization of Lithium-ion Batteries (LIBs), the research has now been focused in increasing functionality, safety and cost-effectiveness to meet the future energy and power density requirements, particularly for electric vehicles. In this scenario, the only options remaining is to apply Li metal as the anode for its ultra-high theoretical capacity of 3860 mAh/g. However, the use of Lithium metal in liquid/polymer batteries containing flammable electrolyte has severe safety concern due to lithium dendritic growth. So, a new all solid-state configuration of LIBs (ASSLBs) is considered as "Better Battery" with improved energy density and safety.

Solid State Electrolyte (SSE)

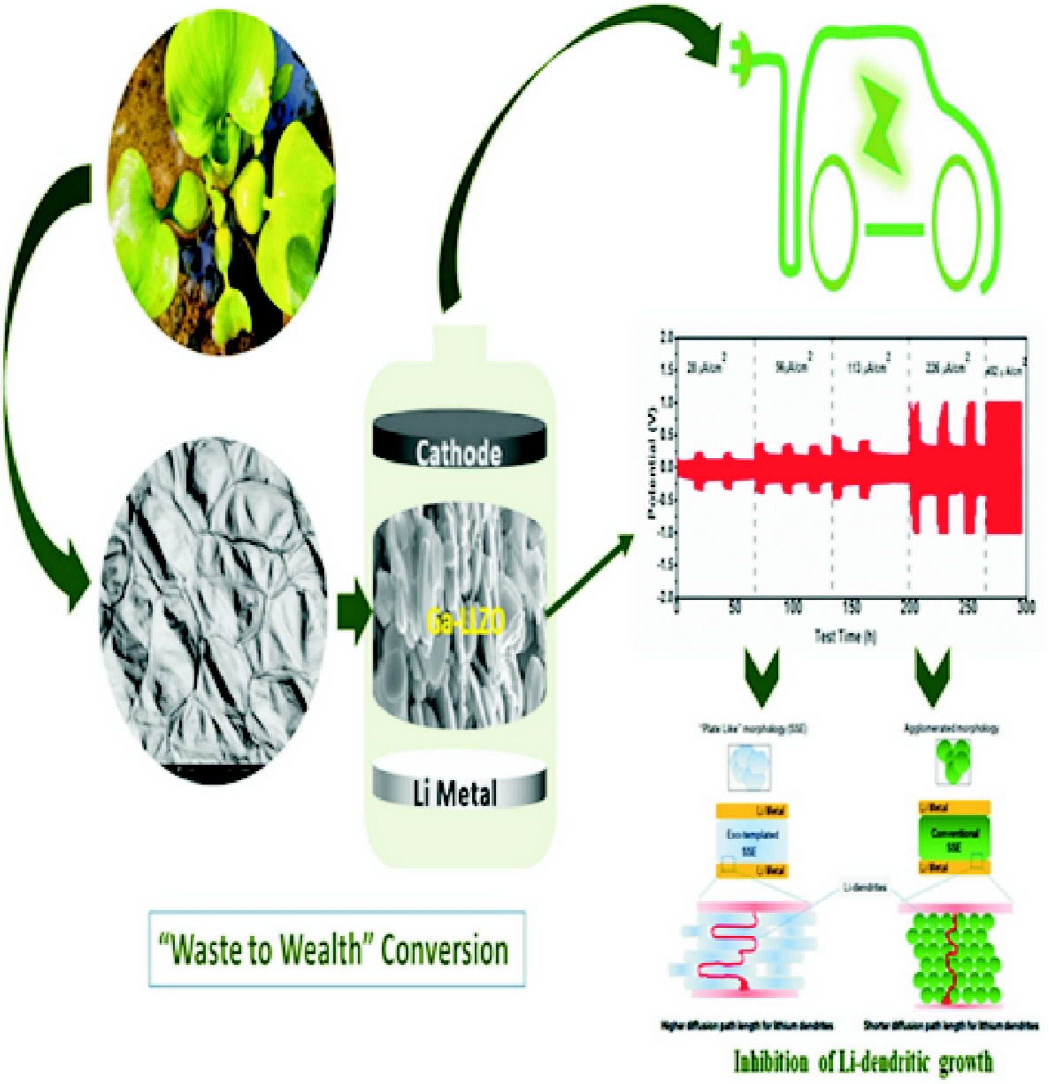
Among several other electrolytes, LLZO ($Li_7La_3Zr_2O_{12}$) garnet has shown exceptional qualities like high Li-ion conductivity (10^{-3}–10^{-4} S/cm at RT), wide electrochemical window (0-6 V vs. Li^+/Li) and extraordinary compatibility with lithium metal. Although, synthesis and stabilization of LLZO is a challenge due to severe lithium loss during high temperature sintering and difficult purification process due to high moisture sensitivity. With addition of that, during cycling, the dendritic growth of lithium metal inside solid state electrolyte remains still a challenge. One of the ways to inhibit dendritic penetration is to engineering of microstructure of electrolyte material and modification of its grain boundaries.

Engineering of microstructure

Bio-templating process has that ability to produce materials with unique and engineered microstructure that can offer plenty of rooms to tune material's properties. Here, we are first time reporting the use of Water Hyacinth bio-waste as a sacrificial bio-template to mimic its inter-cellular structure for developing unique "plate like" microstructure of Gallium doped $Li_7L_3Z_2O_{12}$ ($Li_{6.25}La_3Ga_{0.25}Zr_2O_{12}$, referred as WH-Ga-LLZO) based SSE for its application in ASSLBs. The novel synthesis method resulted in fast ion-conducting cubic phase with bulk lithium-ion conductivity of 3.94×10^{-5} S/cmat 1000°C.

Impeding lithium dendritic migration path

Solid state symmetrical cell with configuration of Li/WH-Ga-LLZO/Li was galvanostatically cycled for continuous 295 h without short-circuit with increasing step current densities from 28 μA/cm^2 to 452 μA/cm^2 where the maximum polarization was found. The pre and post electrochemical analysis revealed that the unique microstructure has successfully inhibited the dendritic migration of metallic lithiumacross the grain boundary. The reason was possibly due to the increase in the diffusion path length of Lithium as schematically illustrated in the figure below.



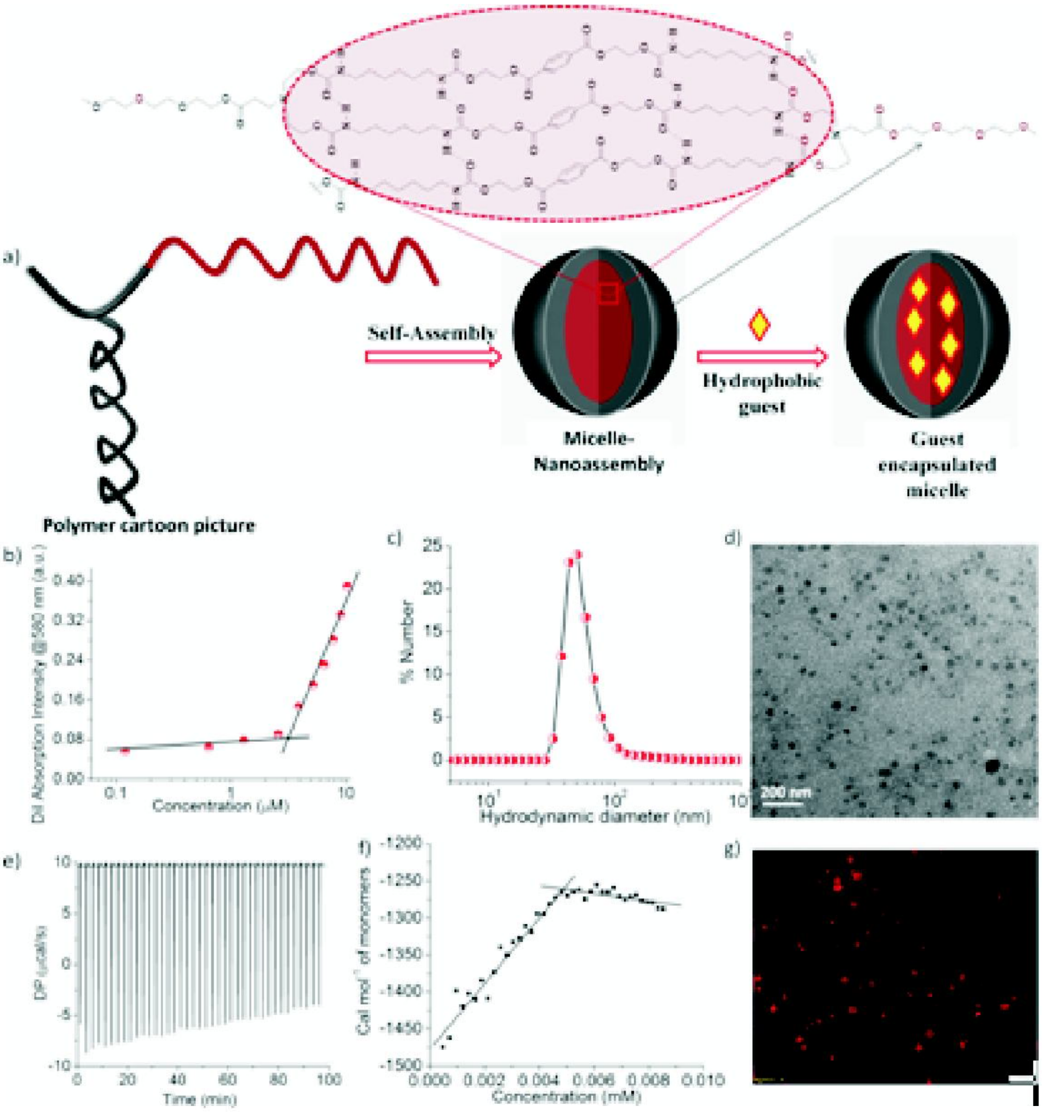
Graphical Abstract

Contributory Paper-135

Supramolecularly cross-linked nanoassemblies of self-immolative polyurethane from recycled plastic waste: High encapsulation stability and triggered release of guest molecules

Subrata Santra and Mijanur Rahaman Molla*[a]
Department of Chemistry,
University of Calcutta,
Kolkata
E-mail: subrata.santrachem@gmail.com

Stabilizing noncovalently encapsulated guest molecules inside a nanoassembly constructed from amphiphilic polymers hasbecome a very challenging effort in the area of targeted drug delivery of biomedical applications. The unwanted disassembly followed by premature release of guest molecules limits their applicability in this field. Hence, designing a robust nanocarrier with efficient noncovalent encapsulation stability would be highly anticipated. Here, recycled plasticwaste is used to synthesize new self-immolative amphiphilic polyurethane equipped with redox responsive disulfide bond, tertiary amine and aromatic moiety on the backbone and periodically implanted triethylene glycol monomethyl ether as a pendant. In aqueous milieu, this polymer self-assembles into smaller micelle type nanoassembly, which shows nanocontainer property by stable encapsulation of hydrophobic guest molecules. In addition to hydrophobic interactions,supramolecular cross-linking in the core by π-π stacking (aromatic moiety) and H-bonding (urethane functionality) interactions brings stability in the micellar nanostructure, which eventually amplifies guest encapsulation stability, which is further confirmed by computational study. As the backbone is integrated with self-immolative redox responsive linker, which can be cleaved in redox environment of cancer cell cytoplasm, a guest release experiment in presence of glutathione (GSH) was tested and it results ~70% guest release in a controlled fashion. Furthermore, tertiary amine present on the polymer backbone leads to the tumor relevant pH (pH~6.5-6.8) regulated charge modulation and formation of positively charged nanoassembly which is very relevant to enhanced cellular internalization as cell membrane hasnegative potential. Thus, utilization of recycled plastic waste to fabricate biodegradable polyurethane based supramolecularly cross-linked stable micellar nanostructure endowed with environment specific surface charge modulation and controlled guest release, we believe, will have significant impact to the ongoing efforts of scientists to find stable nanocarrier with higher encapsulation efficiency for improved chemotherapeutic applications.


a)
Self-Assembly
Hydrophobic guest
Micelle-Nanoassembly
Guest encapsulated micelle
Polymer cartoon picture
b)
DiI Absorption Intensity @560 nm (a.u.)
0.00
0.08
0.16
0.24
0.32
0.40
0.1
1
10
Concentration (μM)
c)
% Number
0
5
10
15
20
25
10^1
10^2
10^3
Hydrodynamic diameter (nm)
d)
200 nm
e)
DP (μcal/s)
10
5
0
-5
-10
0
20
40
60
80
100
Time (min)
f)
Cal mol^{-1} of monomers
-1200
-1250
-1300
-1350
-1400
-1450
-1500
0.000
0.002
0.004
0.006
0.008
0.010
Concentration (mM)
g)

Contributory Paper-136

A comparative study on the protein binding activities of thymol and thymoquinone

Syed Ishmattowaha Parvin, Md. Kalimuddin Mandal,
Md. Maidul Islam and Harun Al Rasid Gazi*
Department of Chemistry,
Aliah University, Action Area IIA/27, New Town,
Kolkata-700 160, India
E-mail: mizan99542@gmail.com

Two phytochemicals, thymol and thymoquinone obtained from *thyme* (*Thymus vulgaris L., Lamiaceae*) and *Nagila Sativa* seed, respectively. Both the phytochemicals show several biochemical activities like anticancer, antimicrobial *etc*[1–3]. In present work we studied the interaction with bovine serum albumin (BSA) with thymol and thymoquinone using spectroscopic and molecular docking techniques. Our studies revealed that both compounds have a high affinity toward BSA and bind to the pocket of BSA. Molecular docking study revealed that both the molecules form hydrogen bonds with amino acids of BSA. UV-Vis absorption spectra revealed that the binding affinities were in the order of 10^3 M^{-1}. Circular Dichroic study showed that conformation of BSA changes during binding. Fluorescence spectroscopic study showed significant quenching on fluorescence intensity of BSA during binding of both the ligand. Temperature dependent binding study reveal that both the bindings were favoured by negative enthalpy and positive entropy changes. Thermodynamic study showed the overall binding free energies are composed of several free energy components.

References

1. Y. M. Yu, T.-Y. Chao, W. C. Chang, M. J. Chang and M. F. Lee, Thymol reduces oxidative stress, aortic intimal thickening, and inflammation-related gene expression in hyperlipidemic rabbits. *J. Food Drug Anal.,* 2016, **24**, 556-563.
2. N. Didri, L. Dubreuil and M. Pinkas, Activity of thymol, carvacrol, cinnamaldehyde and eugenol on oral bacteria. *Pharm. Acta Helv.,* 1994, **69**, 25-28.
3. R. Aeschbach, J. Loliger, B. C. Scott, A. Murcia, J. Butler, M. Halliwell, et al., Antioxidant actions of thymol, carvacrol, 6-gingerol, zingerone and hydroxytyrosol. *Food Chem. Toxicol.,* 1994, **32**, 31-36.

Contributory Paper-137

Rate of reaction under the influence of Microwave Radiation

Aakash Gupta[a] and Debasis Jana[b]
[a]Department of Chemistry,
Indian Institute of Technology, Bombay,
Bombay
[b]Department of Chemistry,
Ramakrishna Mission Vidyamandira
E-mail: guptaaakash6941@gmail.com

In various photochemical reactions, electromagnetic radiations in the range of UV-vis are widely used and the rate of the reactions is generally faster than any other thermal reactions. The electromagnetic radiation in the range of 200–800 nm (UV-vis) has sufficient energy to excite the electrons from one molecular orbital to another. But in the presence of Microwave radiation, the rate of the reaction is also enhanced very much though it is unable to break bonds by excitation of electrons to higher MO. It can only change the rotational state of the molecule by changing the J value. In the presence of water as a solvent, the water molecule moves to its higher excited state and then it returns to the ground state by radiating heat that provides the activation energy of the reaction. But many microwave-assisted solvent-free organic synthesis implies that the above is not the only reason. There are other various reasons for such an increase in reaction rate. Due to the interaction between microwave and molecule the rotation speed of the molecule changes giving the idea of a collision between the molecules in the proper orientation according to collision theory. In presence of a magnetic field and due to interaction with microwave radiation the spin state of the electron. These two may be the cause of the increase in the rate of the reaction under the influence of microwave radiation.

References

1. Satoshi Horokoshi and Nick Serpone, Microwave frequency effects in organic chemistry, *Mini-Reviews in Organic Chemistry*, 2011, **8**, 299-305.
2. Madhvi A. Surati, Smita Jauhari and K. R. Desai, A brief review: Microwave-assisted organic reaction, *Archives of Applied Science Research*, 2012, **4(1)**, 645-661.
3. Kevin D. Raner, Christopher R. Strauss, Ferdinand Vyskoc and Luci Mokbel, A comparison of reaction kinetics observed under microwave irradiation and conventional heating, *J. Org. Chem.*, 1993, **58**, 950-953.

Contributory Paper-138

From fluorogen to fluorophore by elucidation and engineering of ultrafast excited state phenomena of a Schiff base

Souradip Dasgupta[a], Shrobona Banerjee[b], Sharmistha Das[a] and Anindya Datta*[a]
[a]Department of Chemistry,
Indian Institute of Technology Bombay,
Mumbai, Maharashtra, India
[b]Department of Chemistry,
Indian Institute of Science Engineering and Research Bhopal,
Bhopal, Madhya Pradesh, India
E-mail: adutta@iitb.ac.in

Ultrafast dynamics of Schiff bases has drawn significant interest over the past few decades. Torsional motion coupled with rapid proton transfer have been shown to be the major non radiative pathways contributing to their very small fluorescence intensity and lifetimes. In the present study, excited state processes of a Schiff base, salampy, have been probed and modulated in two steps: deprotonation of the phenolic hydrogen using KOH and its complexation with Zn^{2+} and Al^{3+}. In both the cases the newly formed species undergoes a slower decay as compared to the freebase ligand. The locally excited enolic form of salampy undergoes a barrierless ultrafast ESIPT to yield the relatively more emissive cis keto excited state with a lifetime of tens of picoseconds[1]. Abstraction of phenolic H eliminates the possibility of ESIPT and generates an emissive state that resembles the cis keto form with the exception that the proton is not present on the imine nitrogen[2,3]. This species is stabilized by solvation and conformational relaxation to yield a relatively stronger emissive state which decays in 800 ps[4]. Complexation with metals hinders these non radiative processes i.e. ESIPT and torsional motion resulting in an increase in lifetime to 6 ns and 9 ns for Zn^{2+} and Al^{3+} complexes respectively. π-π stacking has been inherently one of the major non radiative pathways which quenches emission in metal complexes of this type[5]. Inhibition of π-π stacking was achieved by chemical modulations in Zn complexes; by formation of bridge bonds in one case and orthogonal orientation of the stacking units in another. The two Zn^{2+} complexes have almost similar fluorescence lifetimes and quantum yields. The Al^{3+} complex is more emissive, possibly because of formation of more rigid complexes.

References

1. W. Rodríguez-Córdoba, J. S. Zugazagoitia, E. Collado-Fregoso and J. Peon, *J. Phys. Chem. A*, 2007, **111**, 6241-6247.

2. M. Zióƚek, M. Gil, J. A. Organero and A. Douhal, *Phys. Chem. Chem. Phys.*, 2010, **12**, 2107.
3. S. Dasgupta, A. Chowdhury and A. Datta, *J. Indian Chem. Soc.*, 2021, **98**, 100122.
4. S. Dasgupta, S. Banerjee, S. Das and A. Datta, *Phys. Chem. Chem. Phys.*, , DOI:10.1039/D1CP02540F.
5. T. Khan and A. Datta, *J. Phys. Chem. C*, 2017, **121**, 2410-2417.

Contributory Paper-139

Active interface engineered oxygen electrocatalysts for electrochemical energy applications

Narugopal Manna[a,b] and Sreekumar Kurungot*[a,b]
[a]Physical and Materials Chemistry Division,
CSIR-National Chemical Laboratory,
Pune-411 008, India.
[b]Academy of Scientific and Innovative Research (AcSIR),
Ghaziabad, Uttar Pradesh-110 001, India
E-mail: n.manna@ncl.res.in

To overcome the existing limitations related to the oxygen electrokinetics in the electrochemical energy devices such as water electrolyzer (OER), PEMFCs (ORR) and RZAB (ORR and OER), more cost-effective and durable catalysts are required. Therefore, strategic modulation of the required active sites and structural fine-tuning of the catalyst morphologies and functionalities are necessary to effectively overcome many of these existing challenges. The size, shape and compositional tuning of the active centers are promising ways to improve the catalyst performance. In addition, the support morphology plays an important role in effectively meeting the various critical activity deciding factors such as mass transport and active site accessibility. Apart from the morphology, the selected support should have electronic conductivity for better electron transport, structural rigidity, and corrosion resistance for enabling the system to withstand harsh electrochemical conditions. Along with these, considering the cost as well as performance deciding factors, the development of low-Pt, and Pt-free electrocatalysts for ORR and OER applications is also becoming an important thrust area. Moreover, compared to the conventional 1D and 2D structured support materials, the less explored 3D structured supports have the unique advantages of providing better accessible actives sites, which results in improved electrocatalytic performance. In the context of the above mentioned technical challenges, a focused effort has been made, as detailed in the various working chapters of this thesis, to develop a series of new classes of the graphene-based 3D structured electrocatalysts for the oxygen electrochemistry applications. The synthesized catalysts show significantly improved performance compared to the state-of-the-art catalysts for the respective reactions. The relevant morphology of the 3D graphene also provides unique structural integrity. In addition, the doping of nitrogen into the 3D framework of the graphene sheets provides efficient anchoring sites for the uniform and well-anchored dispersion of the desired active sites. Furthermore, the stable morphology of the 3D support with its N-doped centers improves the metal-support interaction and thus the designed systems are found to be surviving well under the harsh electrochemical conditions.

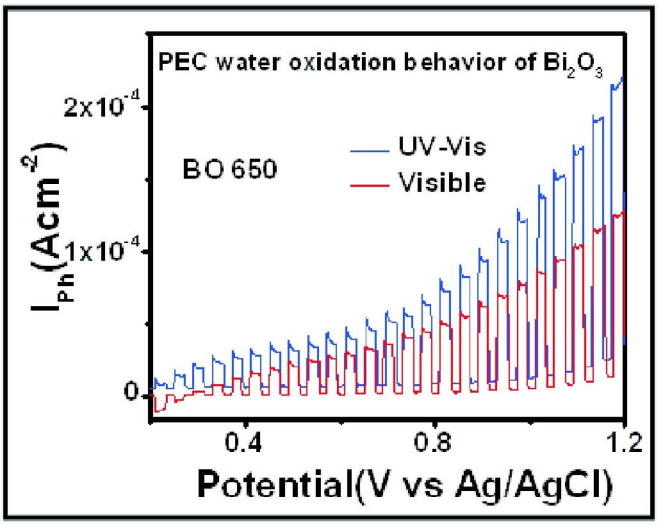
The 3D morphological features of the catalysts are also helpful for achieving better electrode-electrolyte interface formation and, thereby, improved active site utilization. Further, the creation of additional porosity on the 3D support matrix within the range of micro to meso shows another significant advantage of achieving the formation and dispersion of nanometer-sized alloy nanoparticles on the support surface.

Contributory Paper-140

Optimization of growth condition of n-type Bi_2O_3 semiconductors for improved photoelectrochemical water oxidation

Sangeeta Ghosh[a], **Sukumar Kundu**[b] **and Chinmoy Bhattacharya***[a]
[a]Department of Chemistry,
[b]Department of Metallurgy and Materials Engineering,
Indian Institute of Engineering Science & Technology,
Shibpur, Howrah-711 103, West Bengal, India
E-mail: chinmoy@chem.iiests.ac.in

Photoelectrochemical (PEC) water splitting has been considered a promising route for the production of hydrogen (H_2) applying for free solar energy. To produce H_2, PEC systems have great advantages of simple process steps and very low environmental burdens. Bi_2O_3 is a very promising semiconductor with a moderate bandgap of 2.65 eV for PEC water oxidation. The present work describes the development of bismuth (III) oxide (Bi_2O_3) semiconductor (SC) using $Bi(NO_3)_3$ as a precursor followed by annealing in air at various temperatures (200–800°C). Physico-chemical and photocatalytic experiments suggested that the optimized Bi_2O_3 demonstrates highest photo-activity in degrading Rhodamine B target pollutants. The sample annealed at an optimized temperature of 650°C exhibits the highest photo-current of 186 $\mu A\ cm^{-2}$ for $H_2O \rightarrow O_2$ oxidation reaction (in 0.1 *M* Na_2SO_4 - pH7, PBS), at 1.23 V vs. NHE under illumination of 100 mW cm^{-2}. Electrochemical impedance spectra (Mott-Schottky) analysis confirms n-type conductivity for the semiconductors.



References

1. H. S. Park, K. E. Kweon, H. Ye, E. Paek, G. S. Hwang and A. J. Bard, *J. Phys. Chem. C*, 2011, **115**, 17870-17879.
2. P. Hajra, S. Kundu, A. Maity and C. Bhattacharya, *Chem. Engg. J.*, 2019, **374**, 1221-1230.

Contributory Paper-141

Synthesis and characterization of bioactive glass ceramics using nano materials

Tamal Kanti Ghosh, Sujan Kumar Chakrabarti and Sudip Kumar Das
Department of Chemical Engineering,
University of Calcutta,
Kolkata, India
E-mail: tkgcrnn_rs@caluniv.ac.in
sujan.chakrabarti@gmail.com
skdchemengg@caluniv.ac.in

Bioactive glass and glass ceramics materials are used in the medical field as they undergo a specific surface reaction when implanted into the body leading to the formation of a bond between the tissues and material, i.e., hydroxycarbonate (HCA) apatite layer. Nano-Zirconia containing bioactive glass-ceramics (NZGC) have been accepted as trusting bone implants in clinical applications due to their chemical stablity, high mechanical properties, and hydroxycarbonate apatite (HCA) formation capability. The bioactive glass-ceramics have been prepared using NanoSiO$_2$-NanoAl$_2$O$_3$-CaO-CaF$_2$-P$_2$O$_5$-NanoZrO$_2$ systems by melt-quenching technique. The glass-ceramics samples were characterized by differential thermal analysis (DTA) for thermal behaviour and crystallization kinetics, X-ray diffraction analysis (XRD), and the change in surface morphology was determined by scanning electron microscopy with energy dispersive spectroscopy (SEM with EDS) along with Fourier transform infrared spectroscopic (FTIR) techniques. The XRD result showed that the sintered samples crystallized and the fluorapatite phase was obtained as the main crystalline phase along with the wollastonite phase. *In vitro* bioactivity was carried out for biological properties. HCA layer was obtained on the surface of the samples after 28 days of immersion in simulated body fluid (SBF) solution. Cytotoxicity test confirmed that all samples were not cytotoxic.

Contributory Paper-142

Fabrication of Bi oxide layer supported WO_3 photoanode for intensification of photoelectrochemical water oxidation

Debasish Ray and Chinmoy Bhattacharya*
Department of Chemistry
Indian Institute of Engineering Science & Technology, (IIEST),
Shibpur, Howrah-711 103, West Bengal, India
E-mail: cbhattacharya.besus@gmail.com
debasishray888@gmail.com

Reliance on the burning of fossil fuels as the primary energy resource mainly represents a significant driver of anthropogenic changes to the planet. Metal oxide semiconductors are considered the most promising materials for harnessing solar energy to convert the earth-abundant precursors such as H_2O to a carbon-neutral energy source to meet the above concern. Tungsten-based oxides turn out to be enchanting materials due to their paramount characteristics, such as appreciable small band gap energy with suitable band edge position & less prone to photo corrosion in different media inclusion with the low hole diffusion length. The construction of hetero-structures is an excellent strategy to achieve efficient charge separation and improved photocatalytic activity. The present study describes the preparation of Tungsten Based oxide semiconductor (SC) via the drop-cast method using tungstate precursors. Thin films were prepared over a pre-cleaned FTO-coated glass substrate using ethylene glycol as a solvent, followed by annealing at 600°C for 4 hrs. This work describes the drop cast of Bi_2O_3 on WO_3 film; this way, a WO_3/Bi_2O_3 heterojunction is obtained. The absorption spectrum measures 2.8 eV to 2.6 eV bandgap for pure and bi-layered thin film. The prepared bi-layer semiconductor films exhibit significant photoelectrochemical activity and long-term stability in terms of oxygen evolution reaction from water ($H_2O \rightarrow O_2$). The highest photo-current of 610 $\mu A/cm^2$ at an applied bias of +1.0 V (vs Ag/AgCl) under the illumination of 100 mW/cm^2, which is more than 3.0 fold compared to the pure tungsten oxide (200 $\mu A/cm^2$) thin-film under similar condition. Nyquist analysis confirms the better charge transfer resistance for modified thin film. The Mott-Schottky analysis revealed the n-type semi-conductivity of both pure and bi-layered thin films. This work demonstrated that adding calcium is a facile strategy to enhance the photocatalytic activity of tungsten oxide.

References

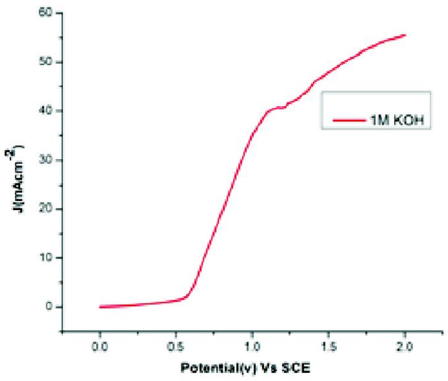
1. S. Sun and W. Wang, *RSC Adv.*, 2014, **4**, 47136-47152.
2. Y. Ma, Z. Wang and Y. Jia, *Carbon.*, 2017, **114**, 591-600.

Contributory Paper-143

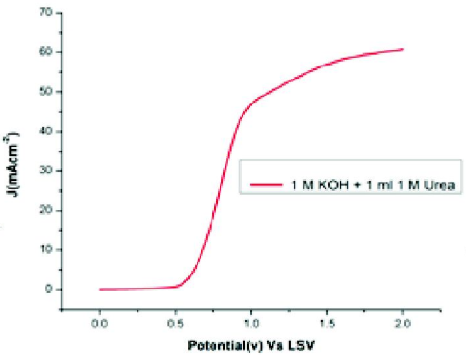
Electrochemical oxidation of urea on synthesized copper oxide nano-particles supported by graphite carbon electrode

Anupam Chowdhury, Rabiul Islam and Swapan Kumar Bhattacharya*
Jadavpur University,
Kolkata
E-mail: achowdhury.chem@gmail.com

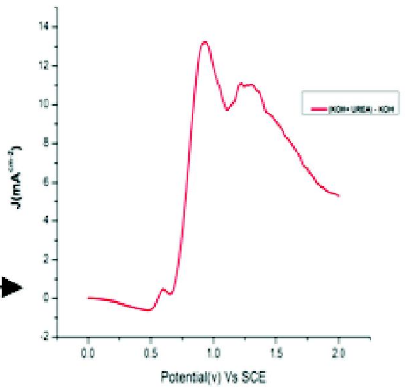
Urea in water, generated from different sources like human, animal, fertilizer, causes degradation of environment. Urease generated by micro-organisms decomposes into toxic ammonia which creates serious health problems. Urea which constitutes about 10 mass percentages of waste waters can be an efficient alternative energy resource. Its oxidation at the anode helps the synthesis of H_2 at the cathode from aqueous solution in an electrolyte cell. Efficient earth-abundant non-noble metal electro-catalyst is therefore the need of the day. For this, CuO nanoparticles are synthesized using wet chemical route and characterized. The use of the synthesized material by deposition on graphite carbon electrode reveals oxidation of urea along with evolution of oxygen in aqueous alkali. The contribution of urea oxidation to the total current density is obtained by subtraction of the blank current, i.e. current in absence of urea from the total when urea is present. After subtraction the current density shows two peaks of urea oxidation for each concentration. The linear plot of peak current density versus concentration signifies successful separation of contribution of urea oxidation from the total current density arising due to simultaneous urea and water oxidation. The high value of current density (15 mA/cm^2) for oxidation of ureareveals significant oxidation of urea. The current density increases with increase of the concentration of urea, indicating urea can be used as a suitable fuel in urea Fuel cell.



LSV curve for 1M KOH solution



LSV curve for 1 M KOH in presence of 1ml 1M urea solution



LSV curve plotted after subtraction of the blank current density (urea absent) from the total current density(urea present

Contributory Paper-144

Organocatalytic approch for the synthesis of naphthalene fluorescent probe via 1,5-intramolecular hydrogen transfer and their biological studies

Madan Sau
National Institute of Technology, NIT Jamshedpur,
Jamshedpur, Jharkhand
E-mail: sau.madan95@gmail.com

Herein we report an organocatalytic synthesis of highly fluorescent naphthalene derivatives through 1,5-intramolecular hydrogen atom transfer. This method produces a wide range of novel naphthalene derivatives in good to excellent yields. This transformation features neat and mild reaction conditions under air, high substrate tolerance along with atom economy. Additionally, this protocol highlights the unprecedented use of DBU for the intramolecular hydrogen transfer reaction where oxidation and reduction occurred in one-pot via an organo-catalytic approach. The synthesized compounds exhibit good fluorescent properties which are utilized in cytotoxic studies and cell imaging studies of colon cancer cell line CT26.

Contributory Paper-145

Synthesis and characterization of 1,2-disubstituted imidazole derivatives as potent inhibitors of Mycobacterium tuberculosis

Afra Quasar Nadaf
K. L. E. Society's P. C. Jabin Science College, Hubli,
Karnataka
E-mail: afraquasar@gmail.com

A multi-step synthetic protocol was employed for the synthesis of (2*Z*)-2-((*E*)-4-(benzylideneamino)phenyl)-3-(1-methyl-1*H*-imidazol-2-yl)acrylonitrile derivatives. The synthesized pharmacophores were characterized by using ^{1}H NMR, ^{13}C NMR, FT-IR and GCMS. The title compounds were screened for anticancer and antitubercular activity. Amongst all the compounds BIA-3, BIA-7 and BIA-13 appeared promising with a MIC value 0.2 to 0.4 µg/mL whereas the other compounds have also exhibited good activity with lower MIC values than the standards. Docking study was performed to check their binding interaction and to deduce the possible mechanism of action involved in the inhibition process.

Contributory Paper-146

Bifunctional catalysis of water splitting reaction by graphite carbon supported synthesized NiO, NiS, NiSe nanoparticles

Mousumi Mondal
Jadavpur University,
Kolkata
E-mail: mousumimondal4495@gmail.com

Plotting the roadmap of future “renewable energy highway” requires drastic technological advancement of devices like electrolysers and fuel cells. Technological breakthrough is practically impossible without advanced fundamental understanding of interfacial energy conversion processes, including electrocatalytic water splitting. Particularly challenging is the oxygen evolution reaction which imposes high demands on the long-term activity of electrocatalysts and electrode support materials. Water electrolysis driven by renewable energy can produce clean energy source hydrogen, but its efficiency remains low, in part because of slow kinetics at the anode for the oxygen evolution reaction (OER). Hydrogen can be produced in a clean way from water by its electrochemical splitting. Water electrolysis consists of two half-reactions, of which the oxygen evolution reaction (OER) is the major source of energy loss. In the case of the alkaline water electrolysis, the spectrum of materials that are stable under the conditions of the OER is significantly broader. In this project, we present synthesis, characterization, and electrochemical portrayal of nickel oxide, nickel sulfide and nickel selenide (NiO , NiS, NiSe) as earth abundant low-cost electrocatalysts for electrochemical water splitting. These electrocatalysts have been characterized using powder X-ray diffraction (XRD) and scanning electron microscopy (SEM). These catalysts show superior OER catalytic performance and excellence stability in alkaline medium. The results of the OER reactions in presence of these three catalysts are better than those of benchmark Ni-based and even noble metal-based electrocatalysts. The continued oxygen generation for several hours reveals the long-term stability and activity of NiO , NiS, NiSe electrocatalysts toward OER and hydrogen generation toward HER. The study reveals that NiSe is the best catalyst in both OER and HER and thus acts as an excellent bifunctional catalyst. This development provides an attractive non-noble metal, highly efficient and stable electrocatalyst toward OER.

Contributory Paper-147

Fabrication of Zn(II) based 2D MOF as effective sorbent for the estimation of dyes

Taposi Chatterjee
Aliah University, Newtown,
Kolkata, West Bengal
E-mail: taposigts89@gmail.com

A Zn(II) bearing two-dimensional (2D) metal–organic framework (MOF) of [Zn2(muco)2(4-nvp)2]•CH3OH (1) has been prepared at room temperature by slow diffusion method. The prepared MOF has been structurally characterized by single crystal X-ray diffraction (SCXRD) technique. The compound 1 constructs a three-dimensional (3D) supramolecular network by the combination of hydrogen bonding and $\pi\cdots\pi$ interactions. Hirshfeld surface analysis has also been carried out to investigate the impact of non-covalent interactions in crystal packing. Furthermore, the synthesized compound 1 has been exploited as effective sorbent for the spectrophotometric estimation of cationic and anionic dyes namely, Rhodamin–B (RDB), Rose Bengal (RB) and Eosine-Y (EY). The maximum absorbances (λ_{max}) of the compound 1 with above dyes were measured at 553 nm, 550 nm and 516 nm respectively. The dye RDB follows Beer-Lambert law in the concentration range of 1.0–6.0 μg/mL with correlation coefficient of 0.980; RB follows in the concentration range of 2.4×10^{-4} -1.21×10^{-3} μg/mL with correlation coefficient of 0.999 and EY follows in the concentration range of 0.4–3.0 μg/mL with correaltion coefficient of 0.999. After sorption of dyes, MOF 1 shows a drastic change in its ε_{max} value. The developed method has the potential to be applied for quantitative estimation of the dyes in the real sample analysis.

Contributory Paper-148

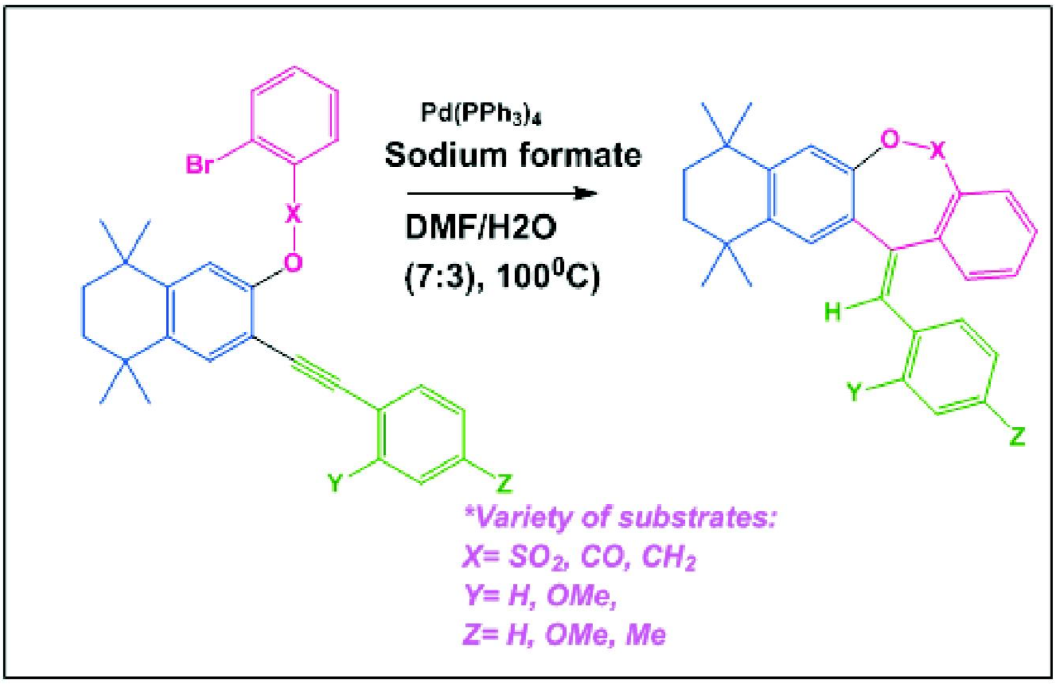
Synthesis of seven membered sultones, oxe-pines, oxe-pinones by palladium-mediated reductive Heck cyclization through retinoid formation

Trisha Mitra[a], Shantanu Chakraborty[a], S. Joardar[b],
Mrinalkanti Kundu*[b] and Brindaban Roy*[a]
[a]University of Kalyani, Kalyani,
Nadia-741 235, West Bengal, India
[b]TCG Lifesciences Pvt. Ltd.,
BN-7, Sector V, Salt Lake City,
Kolkata-700 091, India
E-mail: trishamitra2@gmail.com

The retinoids are a class of chemical compounds that are vitamers of vitamin A or are chemically related to it. The pharmacological uses of retinoids are diverse. Retinoids are used in the treatment of acne, vitamin A deficiency, photosensitivity and have been tested as a treatment for malignant neoplasms. Retinoids affect gene expression through nuclear receptors. They are potent molecules which can affect a variety of fundamental biological processes including cell differentiation and proliferation and apoptosis. However, in spite of their great therapeutic promise, the clinical use of retinoids is still restricted largely to dermatology and some cancers due to the wide range of toxic effects which are associated with the currently available retinoids. The more extensive clinical use of retinoids will occur only if new synthetic analogues with vastly improved therapeutic indices can be developed. Recent advances in the understanding of the molecular mechanisms of action of retinoids suggest that it would be possible to design such retinoids with improved therapeutic indices.

Sultones, oxe-pines and oxe-pinones have emerged as significantly valuable heterocycles that has been widely used as a general building block in the field of medicinal chemistry. Novel sultone functionalized heterocyclic compounds will be particularly useful and desirable in the fields of diversity-oriented chemistry, medicinal chemistry, chemical biology, drug discovery and pharmaceutical industry.

Herein we report a new synthetic protocol for the formation of sultones, oxe-pines, oxe-pinones by palladium-mediated reductive Heckcyclization through retinoid formation.The procedure is straightforward and has been carried out under ligand-free conditions.



**Variety of substrates:*

X= SO_2, CO, CH_2

Y= H, OMe,

Z= H, OMe, Me

References

1. (a) Hiroyuki Yoshimura, Mitsuo Nagai, Shigeki Hibi, Kouichi Kikuchi, Shinya Abe, Takayuki Hida, Seiko Higashi, Ieharu Hishinuma and Takashi Yamanaka, *J. Med. Chem.*, 1996, **38**, 3163-3173;

   (b) Luc J. Farmer, Kristen S. Marron, Stacie S. CananKoch, C. K. Hwang, E. Adam Kallel, Lin Zhi, Alex M. Nadzan, Dave W. Robertson and Youssef L. Bennani, *Bioorganic & Medicinal Chemistry Letters,* 2006, **16**, 2352-2356;

   (c) Hiroki Umemiya, Hiroshi Fukasawa, Masayuki Ebisawa, Laurence Eyrolles, Emiko Kawachi, Ghislaine Eisenmann, Hinrich Gronemeyer, Yuichi Hashimoto, Koichi Shudo and Hiroyuki Kagechika, *J. Med. Chem.,* 1997, **40***,* 4222-4234;

   (d) Susana Álvarez a, Rosana Álvarez a, Harshal Khanwalkar b, Pierre Germain b, Géraldine Lemaire b, Fátima Rodríguez-Barrios a, Hinrich Gronemeyer b and Ángel R. de Lera a, *Bioorganic & Medicinal Chemistry*, 2009, **17**, 4345-4359;

   (e) K. C. Majumdar, Srikantas Samanta and Tapas Ghosh, *Synthesis*, 2012, **44**, 1711-1717;

   (f) S. Joardar, *et al.*, *Synlett,* 2015, **26**, 359-362.

Contributory Paper-149

Synthesis, characterization and biological screening of some antimony(III) complexes with oxygen and sulfur donor ligands

Monika Yadav and H. P. S. Chauhan
School of Chmical Sciences,
Devi Ahilya Vishwavidyalaya,
Takshashila Campus, Khandwa Road,
Indore-452 001
E-mail: monika.svt@gmail.com

Antimony(III) derivatives with oxygen and sulfur donor ligands have been synthesized by the reaction of bis derivative of antimony(III) chloride with sulfur and oxygen donor ligands having molecular formulae; (1) $O_2C_7H_5$, (2) SOC_7H_5, (3) $O_2C_2H_3$, (4) SOC_2H_3, (5) OC_6H_5, (6) SC_6H_5, (7) $O_3C_7H_5$, (8) $SO_2C_2H_3$ in 1:1 *M* stoichiometriy. The series of these newly compounds have been characterized by different physicochemical studies including elemental analysis, melting point and molecular weight as well as spectral studies including IR, NMR (^1H, ^{13}C), powder XRD. The physicochemical data have justified all the elements of expected outcomes. In FTIR spectra the band observed in the region 510–532 cm^{-1} and 282–316 cm^{-1} validated connection with ν(Sb-O) and ν(Sb-S) vibration which confirm the bonding of antimony to oxygen and antimony to sulfur respectively. Powder XRD studies show that these compounds have monoclinic crystal system with nano ranged (9.69–15.69 nm) crystallite size. With the antimicrobial screening test compound (2) has shown maximum zone of inhibition. Thus on the basis of results obtained by previously described techniques, structure of antimony(III) derivatives from compound 01-08 concluded tentatively.

Contributory Paper-150

Experimental and theoretical exploration of sensing and magnetic properties of a triply bridged dicopper(II) complex: The first discrete metal complex to sense picric acid in pure water

Samit Majumder
Department of Chemistry,
Bhairab Ganguly College,
Feeder Road, Belghoria,
Kolkata-700 056, West Bengal, India
E-mail: samitmaj@gmail.com

This presentation reports the syntheses, crystal structures, fluorescence spectra, picric acid (PA) sensing and magnetic properties of a μ-phenoxo-bis(μ-chloro) dicopper(II) compound of composition $[Cu_2L(\mu\text{-}Cl)_2]Cl\cdot4.5\ H_2O$ (**1**), where HL is the [1+2] condensation product of 2,6-diformyl-4-ethylphenol and 2-(2-aminoethyl) pyridine. Compound 1 is water soluble and exhibits fluorescence behaviour in pure water. Interestingly among the various aromatic, non aromatic nitro compounds as well as non nitro aromatic compounds screened, PA specifically quenches the fluorescence intencity of 1 significantly in water, revealing that 1 is a turn-off fluorosensor for PA. The sensing pathways have been investigated by spectral titration, time resolved fluorescence decay and DFT studies. Spectral and theoretical (DFT) studies suggest that the observed fluorescence quenching is associated with ground state (GS) charge transfer as well as electrostatic interactions between 1 and picrate ion. Unaltered fluorescence life time of 1 in the absence and presence of PA strongly suggests that quenching follows a staticmechanism. Nature of binding modes or interactions between the complex 1 and PA was disclosed by the single-crystal structure analysis of the corresponding association complex of composition $[CuII_2L(\mu\text{-}Cl)(H_2O)_2]2Picrate\cdot DMF$ (**2**). The quenching constant (Ksv), association constant (Ka) and detection limit (LOD) of the complex 1 for picric acid was found to be 1.1×105 M^{-1}, 4.64×1010 M^{-2} and 4.8 μM respectively. Variable temperature(2.5 300 K) magnetic susceptibility measurement of the complex 1 reveals antiferromagnetic exchange interaction with $J = -132.40\ cm^{-1}$. The magnetic property has been nicely rationalized in terms of spindensity and magnetic orbitals within broken-symmetry (BS) framework. Compound **1** is the first example of a discrete metal compound to sense picric acid in pure water. Some other interesting aspects have been discussed.

Contributory Paper-151

Proximate and mineral composition analysis on rhizome of *curcuma caesia*

Arvind Kumar Bhardwaj, Milan Hait and Nand Kumar Kashyap
Department of Chemistry,
Dr. C.V. Raman University, Kota,
Bilaspur-495 113, Chhattisgarh, India
E-mail: haitmilan@gmail.com

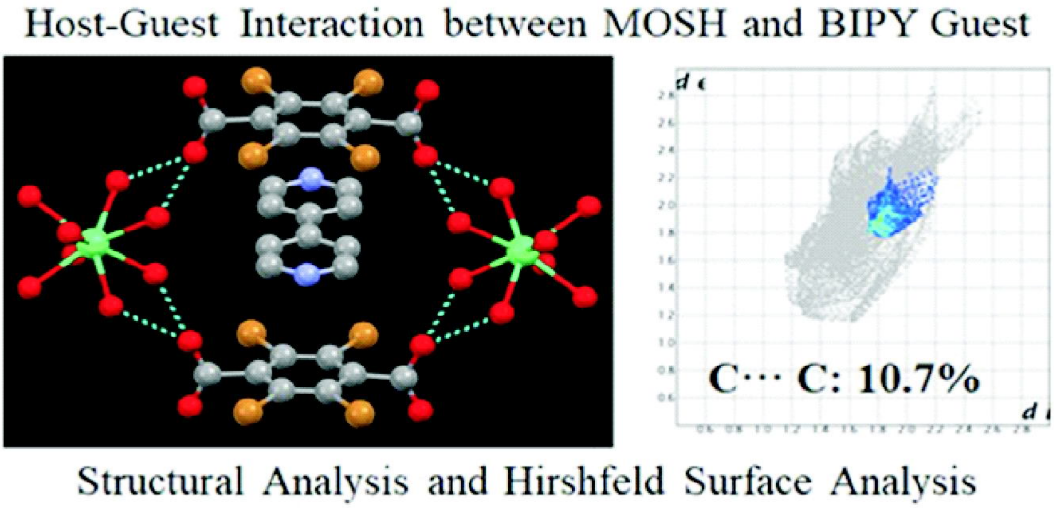
The purpose of this research was to assess the proximate analysis and mineral content of rhizomes of *Curcuma caesia* by employing *in vitro* methods. After cleaning, the rhizomes were allowed to dry at room temperature before being crushed into a coarse powdered form with a mortor and piestle and placed in a container for proximate analysis and mineral determination. The mineral composition was determined using atomic absorption spectroscopic techniques. In the proximate analysis, the following components were found in the sample: moisture content (78.024%), total carbohydrates (19.47%), total ash (3.19%), crude fibre (2.45%), protein content (2.11%) and fat content (0.96%). Also, the concentrations of K (0.42 percent), Mg (0.05 percent), P (0.03 percent), Ca (0.02 percent), and Na (0.01 percent) were all found to be within the range. The current investigation demonstrated that *Curcuma caesia* rhizomes contain high moisture content and vary in mineral composition. *Curcuma caesia* has no harmful characteristics and may be effective in nutritional food supplymentation.

Contributory Paper-152

Investigation of intermolecular interactions between $[Ho(H_2O)_8]^{4+}$ based 3D metal-organic supramolecular host and bipyridyl guest through crystal structure and Hirshfeld surface analysis

Maxcimilan Patra
Department of Chemistry,
Kazi Nazrul University,
Asansol-713 340, India
E-mail: maxcimilan@gmail.com

A new supramolecular metal-organic complex 1,$[\{Ho(H_2O)_8\}^{4+}(TBTA)(bipy)]$ (where H_2TBTA = tetrabromoterephthalic acid and bipy = 4,4′-bipyridyl), has been synthesized hydrothermallyat 100°C by mixing the reactants in stoichiometric ratio. The complex was characterized by single crystal X-ray diffraction (SC-XRD) along with powder X-ray diffraction (PXRD) and other spectroscopic analyses. Structural analysis reveals that 1 crystallized in the tetragonal space group I4 cm and is a mononuclear complex. Ho^{4+} presents octa-coordinated square antiprism geometry having eight coordinated water molecules. Hydrogen bonding interactions between the coordinated water molecules and carboxylate oxygen atoms of TBTA (doubly deprotonated form of H_2TBTA) anions form 3D supramolecular metal organic host (MOSH) having 2D square grid-like supramolecular channels. Guest bipy molecules get stability within the channels through supramolecular $\pi \cdots \pi$ interactions between the bipy and TBTA anions. Hirshfeld surface analysis and corresponding 2D fingerprint plots correlate



with the experimental findings. C···C short contact, corresponding to π···π interactions, contributes around 10.7% to the total surface.

Reference

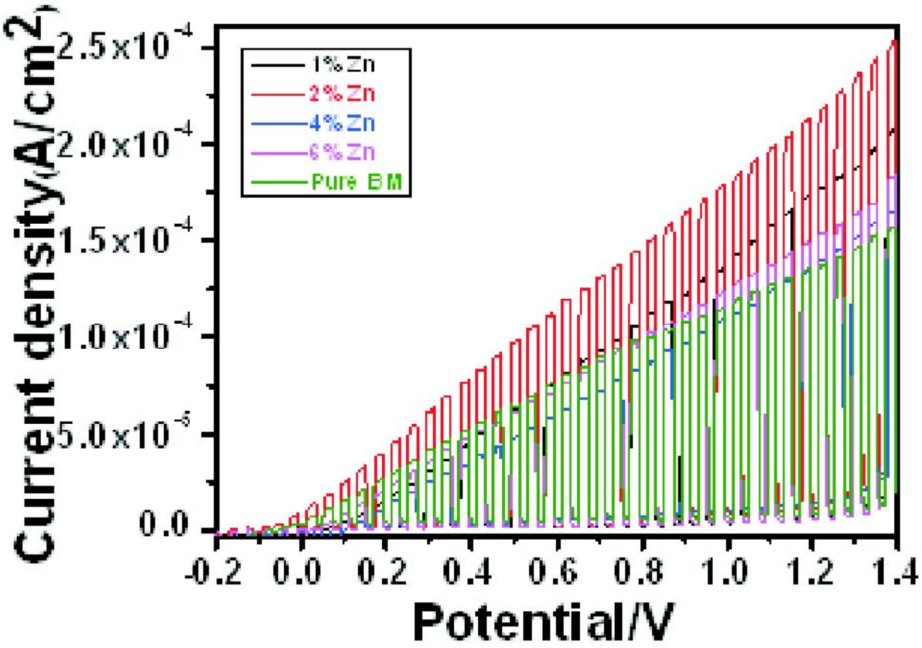
1. Bhattacharjee, *et al*., *Journal of Coordination Chemistry*, 2021, **74**, 1879-1890.

Contributory Paper-153

Optimization of Zn^{2+} modified bismuth molybdate semiconductor for highly efficient photoelectrochemical water splitting

Swarnendu Baduri[a], Surojit Pande[b] and Chinmoy Bhattacharya*[a]
[a]Indian Institute of Engineering Science & Technology,
Shibpur, Howrah, India
[b]Birla Institute of Technology and Science,
Pilani, India
E-mail: chinmoy@chem.iiests.ac.in

One of the greatest challenges in the field of photo-electrochemistry is to develop novel photocatalysts with excellent solar-light-harvesting capacity and separation efficiency of photo-induced charge carriers. Bismuth molybdates are found to be very fascinating materials due to their inimitable characteristics. The narrow band gap energy, high chemical stability and suitable valence band potential of conventional bismuth molybdate makes it a good visible light active photocatalyst but its application is marred by low quantum yield and poor charge separation efficiency. Doping of metal ions in semiconductors alters its surface properties and decreases the recombination efficiency of the photogenerated holes and electron pairs. The construction of heterostructures is regarded as an excellent strategy to achieve efficient charge separation and improved photocatalytic activity. In this work, we have developed



Zn^{2+} modified bismuth molybdate thin film using a simple drop-cast method. Activity of the semiconductors were tested through linear sweep voltammetry under chopped illumination in presence 0.1 M Na_2SO_4 solution for water oxidation and in 0.1 M Na_2SO_3– 0.1 M Na_2SO_4 solution for sacrificial oxidation. The optimized thickness of zinc modified bismuth molybdate yields a photocurrent density of 237 $\mu A/cm^2$ using linear sweep voltammetry[1]. The synthesized samples were characterized by various analytical techniques (SEM, RAMAN). Electrochemical impedance and action spectra suggest significant photon to current conversion efficiencies of the material under UV-vis as well as for visible illumination. In addition, the Zn modified bismuth molybdate photocatalysts maintained good stability atleast for an hour and also most importantly, it is visible light active.

References

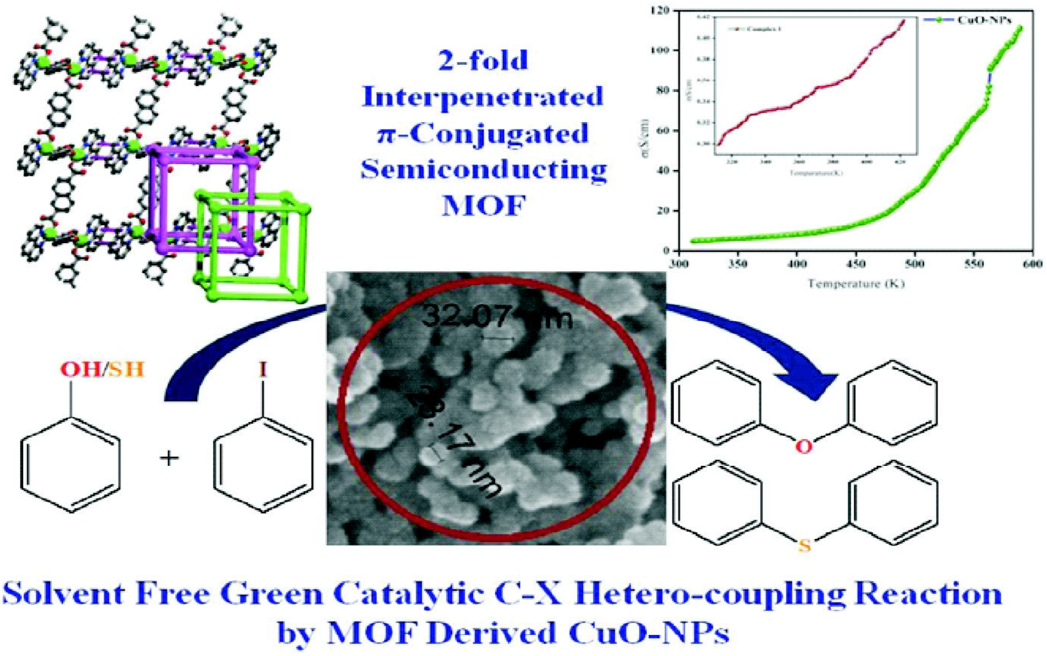
1. G. Zhang, D. Chen, N. Li, Q. Xu, H. Li, J. He and J. Lu, *Appl. Catal. B*, 2019, **250**, 313-324.

Contributory Paper-154

Design of π-Conjugated flexible semiconductive 2D MOF and MOF derived CuO nano-spheres for solvent free C-X (S, O) hetero-coupling catalysis with enhanced conductivity

Soumen Kumar Dubey
Department of Chemistry,
Kazi Nazrul University,
Asansol-713 340, India
E-mail: soumendubey.chem121@gmail.com

A flexible, 2-fold interpenetrated 3D supramolecular structure $[Cu(ndc^{2-})(1,10\text{-phen})]_n$ (where ndc^{2-} = 2,6-naphthalene dicarboxylate and 1,10-phen = 1,10-phenanthroline) comprising neutral 2D metal-organic layers as the basic building block was prepared. Structural study reveals that metal ions are bridged by ndc2-ligands to form 2D coordination layers and the coordinated 1,10-phen moieties are hanging from the layers in the interlamellar spaces. The gliding motion of $\pi\cdots\pi$ stacked layers through 1,10-phen moieties was found to be responsible for the flexibility of MOF and the consequent extended conjugation also renders the semi-conducting behavior of the material. Thermal stability studies revealed that the



framework was pretty stable below 260°C. Additionally, the MOF was characterized by performing adsorption and photoluminescence studies. Further, the MOF was calcined at 650°C to prepare well defined, nearly uniform and spherical shaped CuO nanoparticles (CuO-NPs) with an average size of ~25 nm. Interestingly, CuO-NPs showed around 16 times more conductivity (4.8×10^{-2} S/cm) in relative to the parent MOF (3×10^{-3} S/cm). CuO-NPs induced cross-coupling reactions of alcohols and thiols with aryl halides have been reported. A simple, general, ligand-free and solvent-free procedure for the efficient synthesis of the cross-coupled products in high yield was successfully demonstrated.

Reference

Saha, *et al.*, *Nano-Structures and Nano-Objects,* 2021, **26**, 100756.

Contributory Paper-155

Electrocatalytic oxidation of nitrogen to nitric acid by direct ten–electron transfer using manganese phthalocyanine

Ashadul Adalder* and Uttam Kumar Ghorai
Department of Industrial Chemistry & Applied Chemistry,
Swami Vivekananda Research Centre,
Ramakrishna Mission Vidyamandira,
Belur Math, Howrah-711 202, India
E-mail: iamashadul@gmail.com

Electrochemical nitrogen fixation under ambient conditions is a promising option for the current high energy consumption and greenhouse gas emissions of the nitrogen industry. The energy-intensive Haber-Bosch process produces ammonia, which is the raw material for catalytic oxidization in the classic Ostwald process to generate commercial nitric acid. This two–step energetically non–viable industrial process demands the quest of alternative single step electrolysis from the last century. The quest ends up in optimism when we unravel a ten–electron pathway associated with electrochemical nitrogen oxidation reaction (N_2OR) to nitric acid by using manganese phthalocyanine (MnPc) hierarchical nano–structures (HNs) under ambient condition. The catalyst produces the nitric acid yield of 720 μmol h^{-1} g^{-1}_{cat} at 1.9 V vs. RHE and Faradaic efficiency (F.E.) of 17.32 % @ 1.7 V vs. RHE in 0.01 *M* HCl electrolyte solution. The local co-ordination environment (Mn–N_4) during electrolysis process is confirmed by the X-ray absorption fine structure (XAFS) study. We report a density functional theory (DFT) study which suggests that MnPc has several active sites that can oxidize N_2 gas to form nitric acid. Isotopic labelling experiments and various control experiments validate the source of nitrogen in nitric acid formation. This multifaceted study provides a brand-new insightful understanding of the origin of the active site and catalytic activity of MnPc for N_2OR applications.

Contributory Paper-156

Adsorptive elimination of methylene blue from synthetic medium by raw and acid-modified Bambusa Vulgaris leaves: Batch study

Akanksha Majumder, Koushik Ghosh, Asit Baran Biswas and Sudip Kumar Das*
Department of Chemical Engineering,
University of Calcutta,
92, Acharaya Prafulla Chandra Road,
Kolkata-700 009, India
E-mail: skdchemengg@caluniv.ac.in
drsudipkdas@gmail.com

Bambusa Vulgaris or bamboo leaves (BL) and their two acid (H_2SO_4 and H_3PO_4) treated form SBL and PBL respectively, have been applied as bio-sorbents for the elimination of methylene blue (MB) from the synthetic solution. The bio-sorption has been implemented under different investigational like pH, bio-sorbent quantity, the function of time, initial concentration of MB and temperature. Several kinetic models have been approached to fit the kinetic data, which can be fitted well by the pseudo-second order model, which signifies that chemisorption dominates the bio-sorption. The isotherm data fit well with the Langmuir model with maximum bio-sorption capacity, 181.172 mg/g at 298 K for PBL. The DR (Dubinin-Radushkevich) isotherm also denoted the bio-sorption mechanism controlled by physisorption. Thus, the process indicates chemisorption and physisorption with insignificant bio-sorption energy. The FTIR and ^{13}C NMR outcomes displayed that several functional groups of cellulose, hemicellulose and lignin are associated with MB elimination. The intraparticle diffusion model implies it is not only the rate-limiting step. The overall outcome recommends that bamboo leaves and their acid-treated form be utilized as a low-cost environment-friendly adsorbent to de-pollution effluents laden with primary (cationic) textile dye (MB).

Contributory Paper-157

Tuning photoswitching activity of arylazoimidazoles under visible light

Anirban Dolai, Supriya Bhunia, Sk. Majid Box and Subhas Samanta*

Department of Chemistry,
University of Calcutta,
92, Acharaya Prafulla Chandra Road,
Kolkata-700 009, West Bengal, India
E-mail: dolai.anirban92@gmail.com

The recent growth of the photopharmacology demands the availability of broad variety of photochromic molecules. Heterocyclic azoarenes, such as arylazopyrazoles, have drawn significant attention in recent years. Phoswitching property of arylazoimidazoles (AAIMs) has been known for quite some time[1,2]. However, much attention has not been paid on it probably because of it's poor back isomerization yield and relatively low half-life of cis isomer. All arylazoimidazoles know to date are responsive to toxic UV light for the forward trans-cis isomerization. Here, with the aid experimental and theoretical calculations, we described photoswitching of a broad varity of 2-(arylazo)imidazoles that carry various substitutions at different positions of the aryl ring relative to the azo linker. We establish important structure-property relationships as a function of the nature and location of aryl substitutions. Special attention has been made on the construction of visible light active AAIMs. We have identified an way to approximate cis thermal half-lives of these class of switches simply by calculating CCNN dihedral angle or the N=N bond order, without going for the expensive transition state or excited state calculations. The strategy described herein would greatly facilitate custom design of AAIMs and modulation of photoswitching properties of other arylazoheteroarenes.

References

1. J. Otsuki, K. Suwa, K. Narutaki, C. Sinha, I. Yoshikawa and K. Araki, *J. Phys. Chem. A*, 2005, **109**, 8064-8069.
2. J. Calbo, C. E. Weston, A. J. P. White, H. S. Rzepa, J. Contreras-García and M. J. Fuchter, *J. Am. Chem. Soc.,* 2017, **139**, 1261-1274.

Contributory Paper-158

Development of highly fluorescent sulfur doped graphene quantum dots based fluorescent sensor for the removal of ciprofloxacin from water

Reena Suryawanshi and Kallol K. Ghosh*
*School of Studies in Chemistry,
Pt. Ravishankar Shukla University,
Raipur-492 010
E-mail: reenasuryawanshi1994@gmail.com

The control of environmental pollutants is global concern, recently heteroatom doped graphene quantum dots (GQDs) have been attracted considerable research attention due to their excellent photo luminescent, electrical and properties, excellent thermal chemical stability. Herein, we have developed simple fluorescent-based detection assay for the removal of ciprofloxacin using sulfur doped graphene quantum dots (SGQDs). The SGQDs have been synthesized by hydrothermal method using fructose as carbon source and sulfuric acid as sulfur source. The fluorescence spectra of SGQDs quenched with increasing concentration of ciprofloxacin. The presence of different functional group has been also confirmed by FTIR study. This detection method provides a simple, cost-effective and rapid technique for removal of ciprofloxacin in water sample.

Contributory Paper-159

Polymer based inorganic-organic membranes for desalination of saline water

Mohammad Mujahid Ali Khan[*]
Applied Science and Humanities Section,
University Polytechnic,
Faculty of Engineering and Technology,
Aligarh Muslim University,
Aligarh-202 002, India
E-mail: mujahidchemistry@gmail.com

The polymer-based inorganic-organic membrane was synthesized by sol-gel method and characterized via Scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transformed infrared (FTIR), and Thermogravimetric analysis (TGA). The performance of membrane has been studied in terms of chemical and mechanical stability, membrane thickness, porosity, water uptake and ion-exchange ability and membrane was found to be crystalline in nature with consistent arrangement of particles and no indication of visible cracks on the basis of above results. The membrane potentials measured across the composite membrane in contact with monovalent electrolytes (KCl, NaCl and LiCl), have been found to increase with decrease in concentrations. Furthermore, the synthesized membranes may be applicable for the efficient desalination of saline water.

Contributory Paper-160

Low molecular weight organic gelators

Indrajit Pal*
Department of Chemistry,
Visva-Bharati,
Santiniketan-731 235, India
E-mail: pal.indro2017@gmail.com

Low Molecular Weight Organic Gelator(LMWG), small organic compounds having molecular mass typically less than 3000 strictly belongs to the supramolecular gelator category and is amazingly powerful in immobilizing organic solvents (organogels) and pure water and/or aqueous solvents (hydrogels) at very low concentration of the gelator. An extraordinarily diverse range of compounds can act as LMWGs including bis(ureas) and amides, triazole, tetrazole, saccharides, peptides, nucleobase derivatives, fatty acids, steroids, anthryl derivatives, amino acid derivatives, dendrimers, phthalocyanines and porphyrins etc. Supramolecular metallogels designed with low molecular weight gelators (LMWGs) have attracted great attention in the past few years. LMWGs can play an important role ordered self-assembly processes. The supramolecular self-assembly of LMWGs is associated with non-covalent interactions, which make them more flexible and attractive. The self-assembly of gel materials is initiated as the molecules aggregate into different morphologies in suitable solvent systems by non-covalent interactions, such as π-π stacking, CH-π interactions, hydrogen bonds, hydrophobic interactions, Van der Waals interactions and so on, which lead to the formation of three-dimensional networks. The formation of supramolecular self-assemblies by the interaction of metal ions and small molecules can invoke further versatility. Recent years have witnessed a flow of research work devoted to LMWGs because of their various potential applications in the field of sensing, catalysis, electro-optics/photonics, magnetism, semiconducting device, structure directing agents, cosmetics, foods, conservation of arts, drug delivery, tissue engineering and bio-medical applications etc. In this presentation the role of low molecular weight gelator towards the origination of functional supramolecular hydrogel have been explored.

References

1. P. Terech and R. G. Weiss, Low molecular mass gelators of organic liquids and the properties of their gels. *Chem. Rev.*, 1997, **97(8)**, 3133-3160.
2. P. Dastidar, Supramolecular gelling agents: can they be designed?. *Chem. Soc. Rev.*, 2008, **37**, 2699-2715.

Contributory Paper-161

Biosorption study by Ni(II) resistant *S. cerevisiae*

Jayeeta Banerjee, Ranjan Kumar Basu and Sudip Kumar Das*
Department of Chemical Engineering
92, Acharya Prafulla Chandra Road,
Kolkata-700 009
E-mail: drsudipkdas@gmail.com
skdchemengg@caluniv.ac.in

Ni(II) resistant [5500 mg/L of Ni(II)] *Saccharomyces cerevisiae* AJ208 was developed to remove Ni(II) ions from its aqueous solution at a high concentration. The aim is to develop a sequential batch operation to remove very high Ni(II) concentrations to the allowable limit in the discharge. The *Saccharomyces cerevisiae* AJ208 was characterized using SEM-EDAX, FTIR, ZETA and RAMAN.

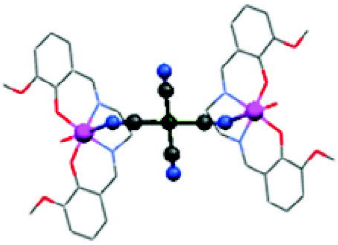
Initially, experiments were carried out to optimize the physical conditions, such as pH, age and volume of inoculum, temperature, and incubation time of the medium. At the optimized operating condition, 96% removal efficiency was observed at initial Ni(II) concentration of 3000 mg/L. Then another two-step re-treatment process was conducted with the optimized operating condition, resulting in Ni(II) concentration of 1.2 mg/L, below the allowable limit as Pollution Control Board prescribed. The *Saccharomyces cerevisiae* AJ208 is a useful adsorbent to clean Ni(II) containing wastewater at high concentrations.

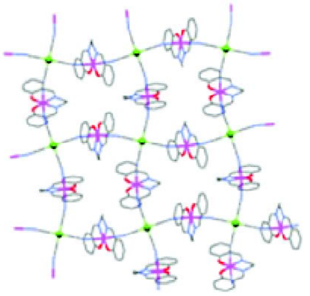
Contributory Paper-162

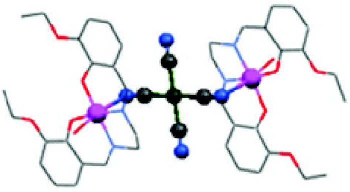
Synthetic strategy, structures and properties of tetracyanometalate bridged transition metal-salen complexes

Susovan Bera and Shouvik Chattopadhyay*
Department of Chemistry,
Jadavpur University,
Kolkata-700 032, India
E-mail: berasusovan97@gmail.com

$[Ni(CN)_4]^{2-}$, $[Pd(CN)_4]^{2-}$ and $[Pt(CN)_4]^{2-}$ may be used as a bridge to connect two or more Metal-salen complexes. Most the complexes are trinuclear, where two *trans* cyanides of a central $[M(CN)_4]^{2-}$ unit bridges two terminal Metal-salen moieties. In few complexes are, however, each of the four cyanides of a $[M(CN)_4]^{2-}$ has been used to bind a M-salen moiety to form a penta-nuclear structure, which is propagating to form 2D sheets with 4,4-square grid topology. Synthesis, structure and the importance of tetracyanometalate bridged transitrion metal-salen complexes have been highlighted here.







Contributory Paper-163

Studies on interaction of azouracils/azoimines with transition metal ions: Biological and analytical applications

Subhasis Ghosh
Department of Chemistry,
The University of Burdwan,
Golapbag, Burdwan-713 104, West Bengal
E-mail: subhasisg456@gmail.com

Azo compounds are very good ligand for transition metals. These have various applications. The azo compounds now are being used in pharmaceutical industry, foods, painting industry etc. They are also used as drugs for cancer cells. The metal complexes of the azo compounds used in medical applications and further research is being continued taking them. Here, the nickel azo complex has shown anticancer activity and the palladium azo complex has shown prominent anti-dengue activity.

Three azouracils, viz. p-carboxyphenylazouracil (L1), p-methoxyphenylazouracil (L2), p-amino phenylazouracil (L3) that have been prepared and characterized by spectroscopic techniques, the structures of L1, L2, L3 have additionally been confirmed by single crystal X-ray diffraction analysis. L1 and L3 have formed complexes with transition metals like Ni and Pd respectively. These are also been characterized by spectroscopic techniques, their structures have additionally been confirmed by single crystal X-ray diffraction analysis also.

Contributory Paper-164

Multicoloured electrochromism and electrofluorochromism in mixed valence-based donor-acceptor-donor compounds

Madhurima Sarkar, Bahadur Sk and Abhijit Patra*
Department of Chemistry,
Indian Institute of Science Education and Research Bhopal,
Bhauri, Bhopal-462 066, Madhya Pradesh, India
E-mail: madhurima18@iiserb.ac.in

Organic electrochromic-electrofluorochromic (EC-EFC) materials have gained distinct attention due to the reflective-emissive dual modes of operation under electric potential for the development of next-generation display devices[1]. However, achieving electrochromism (EC) and electrofluorochromism (EFC) simultaneously in a single molecular system is highly challenging due to the electrochemical instability. In this context, mixed-valence organic systems containing suitable fluorophore bridges have been explored as stable EC-EFC

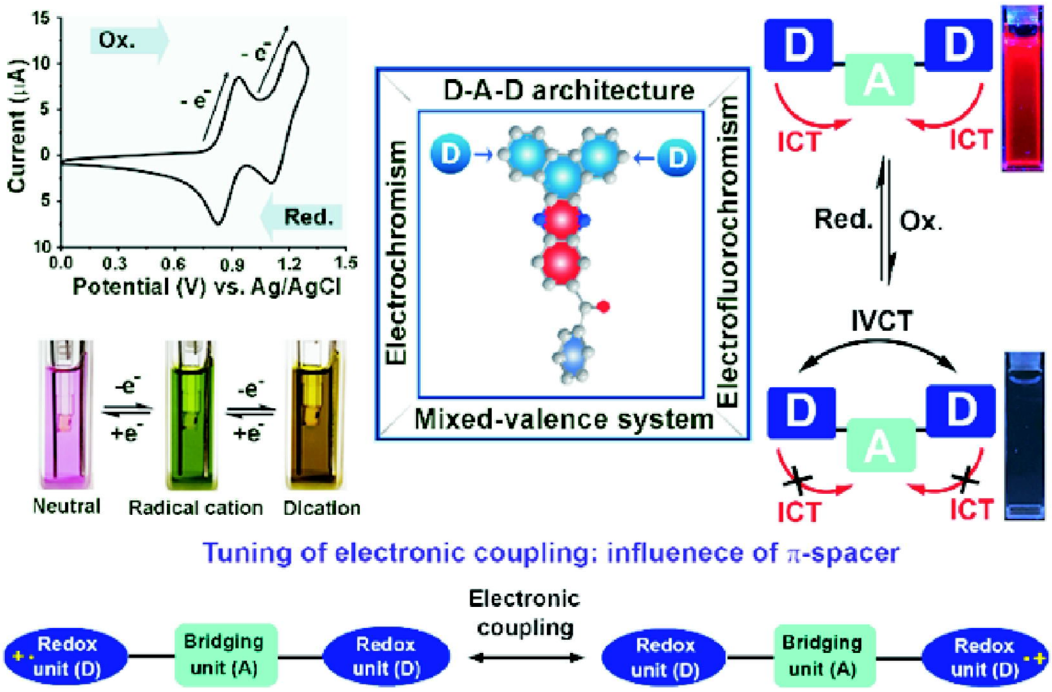


Fig. 1. Schematic illustration of the design strategy involving donor-acceptor-donor (D-A-D) architecture in mixed valence small organic molecule for achieving multistate electrochromism and electrofluorochromism.

materials due to the efficient electronic coupling between the redox centers[2]. Here we have designed mixed-valence multichromophoric organic compounds having donor(D)-acceptor(A) architecture for the development of multifunctional EC-EFC materials[3]. The electrochromic properties of the compounds were studied upon bulk electrochemical oxidation due to the favorable redox window. Along with that, electrofluorochromic property was also investigated via double potential step chronoamperometry experiment. The reversible change in the absorption and fluorescence (ON/OFF) was observed due to the modulation of the intramolecular (ICT) and intervalence (IVCT) charge transfer transition upon electrochemical oxidation of the donor units. Besides, the role of π-spacer on optoelectrical properties and electrochemical stabilities has also been explored by buildinga D-π-A-π-D molecular system using same donor-acceptor units. Electron spin density computation reflects the extent of electronic coupling in the mixed-valence state of the two compounds. The present study opens a promising avenue for achieving the multistate electrochromism-electroflurochromism using donor-acceptor design strategy in all-organic molecular materials[4].

References

1. (a) R. Mortimer, *Chem. Soc. Rev.*, 1997, **26**, 47;
   (b) P. Audebert and F. Miomandre, *Chem. Sci.,* 2013, **4**, 575;
   (c) M. Sarkar, T. Dutta and A. Patra, *Asian J. Chem.,* 2021, **16**, 1.
2. G. Corrente, E. Fabiano, M. Deda, F. Manni, G. Gigli, G. Chidichimo, A. Capodilupo and A. Beneduci, *ACS Appl. Mater. Interfaces,* 2019, **11**, 12202.
3. (a) B. Sk, S. Khodia and A. Patra, *Chem. Commun.,* 2018, **54**, 1786;
   (b) B. Sk, S. Sharma, A. James, A. Kundu and A. Patra, *J. Mater. Chem. C.,* 2020, **8**, 12943.
4. B. Sk, M. Sarkar, K. Singh, A. Sengupta and A. Patra, *Chem. Commun.*, 2021, DOI:10.1039/D1CC05138E.

Contributory Paper-165

Binary solvent-assisted graphene synthesis by direct exfoliation of graphite powder and its cytotoxicity on SiHa cell line

Prabhat Kumar, Purnima Jain and Anjana Sarkar*
Department of Chemistry,
Netaji Subhas University of Technology,
New Delhi, India
E-mail: anjana.sarkar@nsut.ac.in

A cost-effective mass production of pristine graphene nanosheet is still an important challenge to harness its maximum potential in medical sciences. Here, we have used a binary solvent mixture of low dielectric constant (1,2,4-trichlorobenzene, $\varepsilon = 2.24$ and benzylamine, $\varepsilon = 4.6$) to produce a high quantity (0.6 mg/ml) of graphene under ultrasonication without compromising its quality. Obtained sample were characterized through XRD, UV-Vis, Raman, FT-IR, TEM-SAED and cytopotency was evaluated on SiHa cell line. $I_G/I_{2D} < 1.0$ (~ 0.39) was achieved on more than 250 μm^2 area, indicating the uniformity and obtained I_D/I_G ratio was 1.21. No toxicity was found in the case of 24 hr on the SiHa cell line. EC50 computation was 84.90 µg/ml for 48 hr and 62.03 µg /ml for 72 hr. Exfoliated graphene remained stable in binary solvent even after 1 year. The proposed experiment and obtained data can be powerful tools to explore the synergic effect of binary solvent exfoliation in combination to establish graphene as a biomaterial for neuronal network, tissue engineering, drug delivery, and regenerative medicines, to name a few.

Author Index

Invited Lecture

Contributory Paper