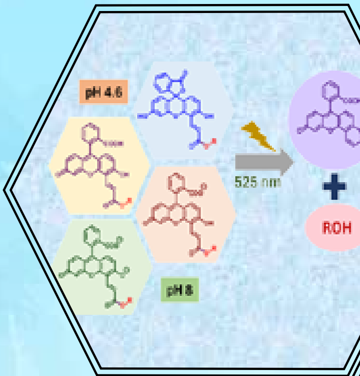
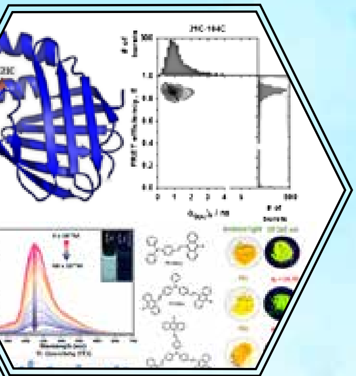
The Proceedings of

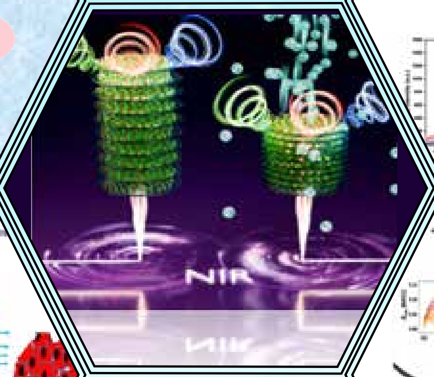
16th National Symposium on Radiation and Photochemistry (NSRP-2025)

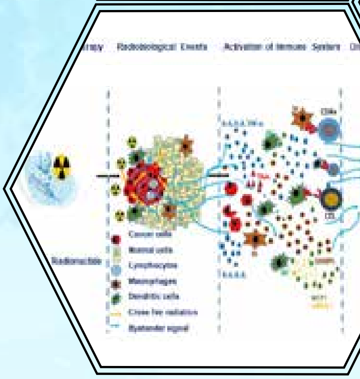


Date:

January 23-25, 2025







Venue:

NISER, Bhubaneswar

Organized by:

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Indian Society for Radiation and Photochemical Sciences (ISRAPS)

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The Proceedings of

16th National Symposium on Radiation and Photochemistry (NSRP-2025)

Venue:

Pathani Samata Auditorium, NISER, Bhubaneswar

Date:

January 23-25, 2025

Organized by:

National Institute of Science Education and Research (NISER)

In association with :

Indian Society for Radiation and Photochemical Sciences (ISRAPS)

Message from the Conveners

We are pleased to announce the 16th National Symposium on Radiation and Photochemistry (NSRP-2025), organized by the Indian Society for Radiation Research and Photochemical Sciences (ISRAPS) and the National Institute of Science Education and Research (NISER), Bhubaneswar, Odisha. The symposium will take place from January 23-25, 2025, at the Pathani Samanta Auditorium. It is our great privilege to be part of this event, which aims to foster scientific discussions on recent scientific advances in the area of radiation chemistry, photochemistry, and allied fields.

NISER Bhubaneswar, established in 2007, is an autonomous research institute aided by the Department of Atomic Energy. The institute focuses on basic sciences education, research, and outreach. It offers integrated M.Sc.+Ph.D. and Ph.D. programs across Biological, Chemical, Computer, Earth, Mathematical, and Physical Sciences. The NISER campus is equipped with state-of-the-art facilities to support academic and research excellence. NISER encourages interdisciplinary research, promotes creativity and innovation, and prepares students for careers in academia, research, and industry. The School of Chemical Sciences, which is collaborating in the organization of NSRP-2025, provides high-quality education and research in both traditional chemistry areas as well as in the interface areas of Biology, Material Sciences and Medicine. NISER's faculty and students are actively engaged in impactful research, and the institute's global collaborations ensure access to the latest scientific advancements. Additionally, NISER contributes to national science policy and fosters a dynamic, innovative research environment.

This symposium brings together experts from prestigious institutions across India, showcasing the country's vast research capabilities in radiation chemistry, photochemistry, spectroscopy, and related areas. The event accentuates the applications of spectroscopy in diverse fields such as materials science, energy, and biophysical chemistry. The participation of institutions from all over India highlights the collaborative spirit and national significance of these scientific disciplines. The successful organization of this event has been made possible by the kind support of the Executive Council, ISRAPS, as well as the faculties of NISER. We would also like to express our heartfelt appreciation for the dedicated efforts of our students, research scholars and staff, whose hard work has been instrumental in making this event a success. On behalf of the organizing committee, we congratulate the entire team for their unwavering commitment and sincere efforts to ensure the symposium is memorable. We extend our gratitude to the National Organizing Committee, the Symposium Organizing Committee of ISRAPS, and the Local Organizing Committee of NISER for their invaluable guidance and support. We are also deeply thankful to our sponsors for their generous financial contributions.

We warmly welcome all participants and sincerely hope that everyone finds this scientific event enriching.

Dr. Beena G. Singh
Convener (BARC)

Prof. Moloy Sarkar
Convener (NISER)

Indian Society for Radiation and Photochemical Sciences

Message from President and Secretary

Dear NSRP-2025 Delegates,

Wish you all a happy, prosperous, and professionally successful New Year 2025!

On behalf of the Executive Council of ISRAPS, it is our privilege to warmly welcome all delegates to the National Symposium on Radiation and Photochemistry (NSRP-2025), scheduled from January 23-25, 2025, at the National Institute of Science Education and Research (NISER), Bhubaneswar. This biennial symposium, organized by ISRAPS with partial support from the Board of Research in Nuclear Sciences, Department of Atomic Energy, serves as a distinguished platform for advancing research in radiation and photochemistry and fostering interdisciplinary collaborations.

ISRAPS is a scientific organization, established in 1984, headquartered at Radiation & Photochemistry Division, Bhabha Atomic Research Centre, Mumbai, INDIA. The society is dedicated to promoting innovative research and knowledge dissemination across diverse domains such as spectroscopy, nanomaterials, atmospheric chemistry, supramolecular chemistry, radiation biology, and beyond. Our initiatives include supporting symposia, publishing bulletins, and organizing one-day discussion meetings at different institutes across India to highlight recent advancements and research contributions.

NSRP-2025 brings together over 150 delegates, featuring invited talks, thesis presentations, and poster sessions. We are confident it will inspire in-depth discussions, foster new ideas, and catalyze collaborative research efforts. To encourage young scholars, ISRAPS confers the Dr. P. K. Bhattacharyya Memorial Award and the Dr. Hari Mohan Memorial Award for outstanding poster presentations in photochemistry and radiation chemistry, respectively. These awards are generously supported by the families of our late founder members. In addition, ISRAPS also sponsors few poster awards during NSRP.

We extend our heartfelt gratitude to the authorities of NISER, Bhubaneswar, for hosting NSRP-2025 and all the organizing committee members for their invaluable contributions and shouldering various responsibilities in organizing this symposium. ISRAPS specially thanks Prof. Moloy Sarkar, Prof. Himansu S. Biswal, Dr. Beena G. Singh and Shri. Amit Kanjilal for their unconditional support in making NSRP-2025 a grand success. Our sincere appreciation also goes to every ISRAPS member for their unwavering support and contributions to the society's endeavors. We request all the researchers to become members of ISRAPS and take active participation in the programs of ISRAPS.

We eagerly anticipate an engaging and fruitful symposium and look forward to continuing our collective pursuit of excellence in radiation and photochemistry research.

Dr. A. C. Bhasikuttan
(President, ISRAPS)

Dr. P. Mathi
(Secretary, ISRAPS)

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Scientific Programme

16th National Symposium on Radiation and Photochemistry

January 23 - 25, 2025
Venue: Pathani Samanta Auditorium, NISER, Bhubaneswar, Odisha

Day 1: Thursday, 23rd January, 2025			
9:00-9:30	**Registration**		
9:30-10:00	**Inauguration**		
Session-I: (10:00-11:00) *Radiation & Photochemistry*			
10:00-10:30	**IT-1**	**Yatender K. Bhardwaj** *BARC Mumbai*	*Radiation induced synthesis and modification of materials*
10:30-11:00	**IT-2**	**Amitava Das** *IISER Kolkata*	*Stimuli-responsive molecular assemblies for theranostic applications*
11.00-11.15	**TEA**		
Session-II: (11:15-13:15) *Radiation Chemistry & Chemical Dynamics*			
11:15–11:40	**IT-3**	**Atanu Barik** *BARC Mumbai*	*Radiation chemistry: An unequivocal tool for studying free radical reaction*
11:40-12:05	**IT-4**	**Pramod Sharma** *BARC Mumbai*	*Ionization of molecules and clusters under influence of laser and electric-discharge pulse*
12:05-12:30	**IT-5**	**Rajib Ghosh** *BARC Mumbai*	*Ultrafast dynamics of singlet fission: mechanistic insights from femtosecond and nanosecond transient absorption spectroscopy*
12:30-13:15	*Session in honour of Prof. J. P. Mittal*		
13:15-14:00	**LUNCH**		
Session-III: 14:00-15:00 *Gas Phase Reaction Dynamics and Atmospheric Chemistry*			
14:00-14:30	**IT-6**	**Aloke Das** *IISER Pune*	*Sequence of protein alphabets prescribes the secondary structures of peptides: A comprehensive picture from condensed and gas phase studies*

14:30-15:00	**IT-07**	**Sachin S. Gunthe** *IITM*	*Oxidation unveiled: Bridging atmospheric chemistry and human physiology*
15:00-16:30	**Poster Session I (PC 01-PC 34) & TEA**		
Session-IV: 16:30-18:00 *Supramolecular Chemistry & Applications*			
16:30-17:00	**IT-8**	**A. Srinivasan** *NISER Bhubaneswar*	*Porphyrins & its analogues: Application as a chemosensor*
17:00-17:30	**IT-9**	**Jyotirmayee Mohanty** *BARC Mumbai*	*Macrocyclic host-based functional supramolecular assemblies: Applications in catalysis, separation, and therapeutics*
17:30-18:00	**IT-10**	**Suhrit Ghosh** *IACS*	*Redox-activable heavy atom free photodynamic therapy*
18:00-19:00	**ISRAPS AGBM**		
19: 30:	*DINNER*		

Day 2: Friday, 24th January, 2025			
Session-V: 9:30–11:15 *Spectroscopy in Sensor Development*			
9:30-10:00	**IT-11**	**Amrita Chatterjee** *BITS Pilani, K K Birla Goa Campus*	*Unlocking the potential of 10,12-pentacosadiynoic acids as multifunctional dual-output chemosensors*
10:00–10:15	**ST-1**	**Suvankar Dasgupta** *NIT Patna*	*Pseudorotaxane, metastable rotaxane and rotaxane-based molecular switches for anion responsive studies*
10.15-11.15	**OP1-OP6**	**Oral Presentation**	
11:15-11:30	TEA		
Session-VI: 11:30–13:15 *Frontiers in Radiation and Photochemistry*			
11:30–12:00	**IT-12**	**Juby K Ajish** *BARC Mumbai*	*Radiation induced synthesis of polymeric systems for various biomedical applications*
12:00–12:15	**ST-2**	**Ravi K. Kanaparthi** *Central University Kerala*	*A highly sensitive colorimetric and fluorometric sensor for the detection of cyanide*

12.15-13.15	**OP7-OP12**	**Oral Presentation**	
13:15-14:00	**LUNCH**		
Session-VII: 14:00-16:00 *Ultrafast Spectroscopy*			
14:00-14:30	**IT-13**	**Chayan K Nandi** *IIT Mandi*	*Single molecule spectroscopy of emerging nanomaterials for super resolution optical imaging*
14:30-15:00	**IT-14**	**Jino George** *IISER Mohali*	*Photophysics of hybrid light-matter states*
15:00–15.30	**IT-15**	**Sayan Bagchi** *CSIR-NCL Pune*	*Water-enhanced DES electrolytes for stable zinc-ion batteries*
15.30-16.00	**ST-3**	**Somen Mondal** *ICT Jalna Campus*	*Vision of fundamental proton and electron transfer: Advancing from spectroscopy to bioelectronics*
16:00–16:15	**Technical session** (*ATOS Instruments Marketing Services*)		
16:15–16:30	TEA		
16:30–18:00	Poster Session II (PC 35-PC 76; RC 01-RC 14)		
18:00–19:00	**CULTURAL PROGRAM**		
19:00	*BANQUET DINNER (Cloud Hill Resort)*		

Day 3: Saturday, 25th January, 2025			
Session-VIII: 9:30-11:00 *Radiation Chemistry: Application in Materials and Medicine*			
9:30-10:00	**IT-16**	**R. Puspalata** *BARC Facilities Kalpakkam*	*Role of radiation chemistry in nuclear technology & beyond*
10:00–10:30	**IT-17**	**Kiran K. Sharma** *Shivaji University Kolhapur*	*Study of gold nanoparticles interaction with N, N, N′, N′ –tetramethyl-p-phenylenediamine radical cation using steady state radiolysis*
10:30–11:00	**IT-18**	**Gayathri N. Banerjee** *VECC Kolkata*	*Optimizing ion irradiation techniques to simulate neutron-induced damage in nuclear reactor core materials: Insights from VECC through experimental and simulation studies*
11:00–11:15	**ST-4**	**Rohit Sharma** *BARC Mumbai*	*Radioimmunotherapeutic agents for targeting HER2 over expressing cancers*
11:15–11:30	TEA		

Session-IX: 11:30-13:15 *Spectroscopy in Materials for Energy*			
11:30-12:00	**IT-19**	**Subhadip Ghosh** *NISER Bhubaneswar*	*Facet engineer fortailoring photophysical processes in perovskite nanocrystals*
12:00-12:30	**IT-20**	**Santanu Bhattacharya** *IISER Berhampur*	*Sustainable nanomaterials for solar to chemical energy conversions through complete metal free approach*
12:30-13:00	**IT-21**	**Yatendra S. Chaudhary** *CSIR-IMMT Bhubaneswar*	*Design of intrinsic white light emitting phosphors and their W-LEDs*
13:00-13:15	**ST-5**	**Palas Roy** *IIT Bhubaneswar*	*Resolving the role of solvent polarity, viscosity and hydrogen-bonding in thermally activated delayed fluorescence*
13:15–14:00	**LUNCH**		
Session-X: 14:00 - 16:00 *Spectroscopy in Biophysical Chemistry*			
14:00-14:30	**IT-22**	**Jatish Kumar** *IISER Tirupati*	*Chiral light emitting nanomaterials: From fundamentals to applications*
14:30-15:00	**IT-23**	**Priyadip Das** *SRM Inst. Sci. Technol., Chennai*	*Zn coordinated self-assembled dipeptide based fluorescent nanoparticles faciliate cellular imaging & targeted drug delivery*
15:00-15:30	**IT-24**	**Harekrushna Sahoo** *NIT Rourkela*	*Perturbation of protein conformation and kinetics by polyethylene glycol: a correlation between ensemble and single-molecule approach*
15:30-16:00	**IT-25**	**Hirak Chakraborty** *Sambalpur University*	*Mechanism of membrane fusion: Interplay of lipid and peptide*
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Session-XII: 16:45-17:45	*Concluding session*		
16:45-17:45	**Poster Award Distribution & Concluding Session**		
17:45–18:00	**TEA**		
19: 30:	*DINNER*		

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IT-12	RADIATION INDUCED SYNTHESIS OF POLYMERIC SYSTEMS FOR VARIOUS BIOMEDICAL APPLICATIONS *Juby K. Ajish*
IT-13	SINGLE MOLECULE SPECTROSCOPY OF EMERGING NANOMATERIALS FOR SUPER RESOLUTION OPTICAL IMAGING *Chayan K Nandi*
IT-14	PHOTOPHYSICS OF HYBRID LIGHT-MATTER STATES *Jino George*
IT-15	WATER-ENHANCED DES ELECTROLYTES FOR STABLE ZINC-ION BATTERIES *T. Chowdhury and S. Bagchi*
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IT-20	SUSTAINABLE NANOMATERIALS FOR SOLAR TO CHEMICAL ENERGY CONVERSIONS THROUGH COMPLETE METAL FREE APPROACH *Santanu Bhattacharyya*
IT-21	DESIGN OF INTRINSIC WHITE LIGHT EMITTING PHOSPHORS AND THEIR W-LEDS *Asish K. Dehury, Rajeswari Kainda and Yatendra S. Choudhury*
IT-22	CHIRAL LIGHT EMITTING NANOMATERIALS: FROM FUNDEMENTALS TO APPLICATIONS *Jatish Kumar*
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ST-4	RADIOIMMUNOTHERAPEUTIC AGENTS FOR TARGETING HER2 OVEREXPRESSING CANCERS *Rohit Sharma*
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RC-10	EXPERIMENTAL L- SHELL X-RAY RELATIVE INTENSITIES OF $_{83}$Bi INDUCED BY HIGH-ENERGY B^{q+} IONS *Anil Kumar, Balwinder Singh, Shehla, Deepak Swami, Ajay Kumar and Sanjiv Puri*
RC-11	RADIATION CHEMICAL STUDIES OF THIOFLAVIN T (ThT): AN UNEXPLORED AREA OF RESEARCH *Anand A Sable, Atanu Barik, J. Mohanty and A. C. Bhasikuttan*
RC-12	RADIATION INDUCED SYNTHESIS OF GOLD NANOPARTICLE DECORATED GLYCOPOLYMERS FOR ANTICANCER DRUG DELIVERY *V. S. Patil, J. K. Ajish and K. S. A. Kumar*

RC-13	RADIOLYTICALLY SYNTHESIZED SILICA NANOPARTICLES As A ROBUST FLUOROPROBE FOR SENSING OF Cr (VI): PAPER STRIP-BASED DETECTION AND ANTIOXIDANTS PROPERTIES *Apurav Guleria, Abina Hari, Snehal S. Chiplunkar and Madhab C. Rath*
RC-14	INVESTIGATION OF RADIOLYTIC FORMATION OF VO2 NANOPARTICLES VIA ALCOHOL RADICALS *Sangeeta J. Keny and M. C. Rath*
PHOTOCHEMISTRY POSTERS	
PC-1	DESIGN AND SYNTHESIS OF pH-RESPONSIVE, WATER-DISPERSIBLE N, S-DOPEDRED EMISSIVE CARBON DOTS FOR BACTERIAL IMAGING *A. A. Pinheiro, M. Banerjee and A.Chatterjee*
PC-2	HALOARENE-DERIVED MULTIFUNCTIONAL AMIDES AND SULPHONAMIDES AS POTENTIAL DRUG CANDIDATES *Abinasha Biswal, Laxmi Narayan Sahoo and Satyanarayan Sahoo*
PC-3	SUPRAMOLECULAR HOST-GUEST COMPLEXATION OF AMPHIPHILIC STYRYL DYES WITH CYCLODEXTRIN DERIVATIVES *Supratim Koley, P. R. Gupta, N. Barooah, J. Mohanty and A. C. Bhasikuttan*
PC-4	DICARBATRIPHYRIN(2.1.1) AND ITS CARBACALIX[1]PHYRIN ANALOGUE: STRUCTURE-PROPERTY RELATIONSHIPS AND APPLICATION AS A Fe(III) CHEMOSENSOR *Adrija Kayal, Sourav Ranjan Pradhan and A. Srinivasan*
PC-5	HOW PEG-BASED CROWDERS AFFECT ULTRAFAST ENERGY FLOW IN HEME PROTEINS *Ambika Prasad Kar, S. Majumdar and P. K. Chowdhury*
PC-6	PHOTOPHYSICAL STUDY OF A BENZOTHIAZOLE DERIVATIVE AND ITS INTERACTION WITH CYCLODEXTRIN HOSTS *Ananya Bera and Sharmistha Dutta Choudhury*
PC-7	N-HETEROCYCLIC RESORCIN[4]ARENE CAVITANDS: A VERSATILE PLATFORM FOR DIFFERENT APPLICATIONS *Manini Nayak, Manas Ranjan Swain and Anita Pati*

PC-8	KINETIC INVESTIGATION OF BUTYLAMINE WITH OH RADICALS *Anjli Pal and Balla Rajakumar*
PC-9	SYNTHESIS AND BIOLOGICAL EVALUATION OF FLUORESCENT BENZOISOQUINOLONYL PEPTIDE/ TRIAZOLE CONJUGATED *β*-D-RIBOFURANOSE *Ankita Panda, S. Harsha Vardhan and Nagendra K. Sharma*
PC-10	ULTRAFAST DYNAMICS OF NONRIGID NICKEL PORPHYRIN DIMER *Sucheta Kundu, Arya Roychowdhury, Sankar Prasad Rath and Anindya Datta*
PC-11	FöRSTER RESONANCE ENERGY TRANSFER FROM PYREDIYNE QUANTUM DOTS IN GEL MEDIA *Arulmozhi Puhazhendhi and Soumya Sivalingam*
PC-12	APPLICATION OF POLYMER-INDUCED AGGREGATION OF RHODAMINE 6G FOR SENSING SULFIDE IONS IN WATER *Ayentika Sen, Aruna K. Mora, Alok K. Ray, Asawari D. Rath and Sukhendu Nath*
PC-13	DECIPHERING THE SYNERGISTIC INFLUENCE OF CONJUGATED RHODANINE ACCEPTORS IN D-D′-A FRAMEWORKS FOR PHOTOVOLTAIC APPLICATIONS *Bhuvaneesh Ilango, Collinica Syiemlieh, Marappan Velusamy and Arunkumar Kathiravan*
PC-14	BIO-INSPIRED METAL-ORGANIC FRAMEWORK (MOF) DERIVED MATERIALS FOR ELECTROCHEMICAL APPLICATION *Litun K. Pradhan and J. N. Behera*
PC-15	GOLD NANOTRIANGLE TETHERED MONOSTABLE [2] ROTAXANE FOR SELECTIVE FLUORIDE ANION DETECTION *Chavda Gayatri, Suvankar Dasgupta and Aniruddha Paul*
PC-16	EXPLORING THE SPECIFIC ROLE OF IRON CENTER ON THE CATALYTIC ACTIVITY OF HUMAN SERUM TRANSFERRIN: CTAB-INDUCED CONFORMATIONAL CHANGES AND SEQUESTRATION BY MIXED MICELLES *Rahul Yadav, Atanu Nandy, Asim Bisoi and Saptarshi Mukherjee*
PC-17	EFFECT OF BIMETALLIC NANOCOMPOSITE SYSTEM (Au@ Ag) ON THE ENZYMATIC ACTIVITY MODULATION OF α-CHYMOTRYPSIN *Chinmayee Patra and Moloy Sarkar*

PC-18	THEORETICAL EXPLORATION OF TWO-DIMENSIONAL MATERIALS FOR OPTICAL, THERMAL AND ELECTRICAL PROPERTIES *Dhananjay and Ravi Kumar Kanaparthi*
PC-19	PHOTOPHYSICAL CHARACTERISTICS OF 3-(2,4-DICHLORO-PHENYL)-1-(3-METHOXY-PHENYL)-PROPENONE: EXPERIMENTAL AND COMPUTATIONAL APPROACH *Divya Jattu Gouda, B. Siddlingeshwar and Shivraj B. Radder*
PC-20	SURFACE FUNCTIONALIZED GOLD NANORODS FOR TARGETED PHOTOTHERMAL THERAPY *Rupayana Panda and Jasaswini Tripathy*
PC-21	GAS-PHASE PHOTOLYSIS AND OH REACTION KINETICS OF VINYL METHACRYLATE *Atanu Halder and B. Rajakumar*
PC-22	FLUORESCENT BASED DETECTION OF ANTIINFLAMMATORY DRUGS USING CAPPED CADMIUM SULFIDE QUANTUM DOTS *K. Dhanalakshmi and K. Swarnalatha*
PC-23	MOLECULAR-LEVEL CHARACTERISATION OF THE CHALCOGEN BOND INTERACTION: A CASE STUDY OF THIOPHENE WITH DIMETHYLACETAMIDE *Heena Charaya, Riya Saha, Debabani Ganguly, Amrita Chakraborty and Shamik Chakraborty*
PC-24	OLYDOPAMINE-FUNCTIONALIZED IRON OXIDE NANOPARTICLES: SYNTHESIS, CHARACTERIZATION AND INTERACTION WITH HUMAN SERUM ALBUMIN *Himanshu Shekhar, Priyatama Behera, Monalisa Mishra and Harekrushna Sahoo*
PC-25	BINDING CATIONS AND COUNTER ION'S ROLE IN THE INTERFACIAL WATER NETWORK AROUND DIBENZO-18-CROWN-6 ETHER *Anmol Virmani, A. Saha, M. P. Walavalkar, A. Sharma, S. Sengupta and A. Kumar*
PC-26	PROBING THE INTERACTION MECHANISM BETWEEN COPPER NANOCLUSTER AND CALF THYMUS DEOXYRIBONUCLEIC ACID *Joyoti Ghosh and Moloy Sarkar*

PC-27	LIGHT-INDUCED REVERSIBLE INTERCONVERSION OF FCC Ag_{14}NCS TO HEXAGONAL Ag_7NCS: PARTICLE-ASSISTED REVERSIBLE INTERCONVERSION *Paritosh Mahato, Koushik Mandal, Khokan Paria, Deepak Chopra and Saptarshi Mukherjee*
PC-28	TARGETING AMYLOID FIBRILS VIA MACROCYCLIC TEMPLATED SILVER NANOPARTICLES *Monika Gaur, R. Khurana, N. Barooah, A. C. Bhasikuttan and J. Mohanty*
PC-29	PROTEIN CONFORMATION, DYNAMICS AND FUNCTION: A CORRELATION WITH SHAPE AND SIZE OF MACROMOLECULES *Laxmipriya Prusty and Harekrushna Sahoo*
PC-30	PROBING AROMATICITY WITH SUPERSONIC JET SPECTROSCOPY *Akshay Kumar Sahu, Anant Ram Satpathi, Saiprakash Rout, Laxmipriya Dash and Himansu S. Biswal*
PC-31	DESIGN & FABRICATION OF ECOFRIENDLY R-PE INCORPORATED HYDROGEL STRIPS FOR THE SELECTIVE DETECTION OF Hg^{2+} IN AQUEOUS MEDIA *Manikandan C. and John Prakash*
PC-32	SPECTROSCOPIC INVESTIGATION ON SOLVATOCHROMISM OF 7-AMINOFLAVONE: AN EXPERIMENTAL AND COMPUTATIONAL APPROACH *M. Suhail, N. Fatma, R. C. Joshi, P. Pant and S. Pant*
PC-33	ORIENTATION OF HYDROCARBON CHAINS OF TRIBUTYL PHOSPHATE IN BULK AND INTERFACE OF WATER *Mohini P. Walavalkar, Anmol Virmani, Asmita Sharma, Ankur Saha and Sumana Sengupta*
PC-34	NEW ELECTRON DONOR-ACCEPTOR MOLECULES BASED ON 2-(4H-CHROMEN-4-YLIDENE) MALONONITRILE FOR SENSING AND BIOLOGICAL APPLICATIONS *Gummadi Leela Prabha Anisha and Ravi Kumar Kanaparthi*
PC-35	FACET-SPECIFIC PHOTOLUMINESCENCE BLINKING IN PEROVSKITE NANOCRYSTALS *Mrinal Kanti Panda, Debopam Acharjee, Asit Baran Mahato and Subhadip Ghosh*

PC-36	INTERACTION OF BIOGENIC SILVER NANOPARTICLES WITH BOVINE SERUM ALBUMIN *Madhumita Patar and N. S. Moyon*
PC-37	PHOTOLUMINESCENCE PROPERTIES OF 7-HYDROXYFLAVONE IN AQUEOUS MEDIUM: A FLUORESCENCE ENHANCEMENT STUDY *Nisha Fatma, Sanjay Pant, Nupur Pandey and Mohan Singh Mehata*
PC-38	UNDERSTANDING THE ANTIMICROBIAL ACTIVITY OF IONIC LIQUIDS THROUGH ORGANISATION AND DYNAMICS STUDY OF MODEL MEMBRANES *Liza Pradhan and Lipika Mirdha*
PC-39	DIMENSION-CONTROL $CsPbBr_3$ PEROVSKITE SYNTHESIS BY TUNING Pb(II) COUNTER ANION AND THEIR APPLICATION IN ORGANIC PHOTOCHEMISTRY *Pravat Nayek, Anupam Manna and Prasenjit Mal*
PC-40	HIGHLY SENSITIVE AND COLORIMETRIC DETECTION OF MERCURY IONS IN WATER *R. Surya Sekhar Babu and Ravi Kumar Kanaparthi*
PC-41	FLUORESCEIN AS A PHOTOREMOVABLE PROTECTING GROUP: PROBING pH-DEPENDENT PHOTORELEASE AND APPLICATIONS *Subham Pal and N. D. Pradeep Singh*
PC-42	SURFACE-IMMOBILIZED SILVER NANOTRIANGLES FUNCTIONING AS PORTABLE SENSING PLATFORM FOR BIMODAL DETECTION OF MERCURY (II) IONS *Rajeev Kumar Shandilya and Aniruddha Paul*
PC-43	PHOTOPHYSICAL STUDIES OF PYRENE BASED FLUORESCENT BIOSENSOR INTO LIPOSOMES *H. Dhilshath Raihana and K. Swarnalatha*
PC-44	FACET ENGINEERING FOR DECELERATED CARRIER COOLING IN POLYHEDRAL PEROVSKITE NANOCRYSTALS *Debopam Acharjee, Ayendrila Das, Mrinal Kanti Panda, Manas Barai and Subhadip Ghosh*

PC-45	HYGROSCOPIC BEHAVIOR OF MIXED INORGANIC $NaNO_3$-$Mg(NO_3)_2$ AEROSOLS *Subhash Sarkar, Subhamoy Saha and P. Mathi*
PC-46	CYSTINE-CORED DIPHENYLALANINE APPENDED PEPTIDE-BASED SELF-ASSEMBLED FLUORESCENT NANOSTRUCTURES DIRECT REDOX RESPONSIVE SITE-SPECIFIC CHEMOTHERAPEUTIC DRUG DELIVERY *Suman Nayak, Kiran Das, Subramaniyam Sivagnanam, Shyamvarnan Baskar, Adele Stewart, Dinesh Kumar, Biswanath Maity and Priyadip Das*
PC-47	EFFECT OF TRIETHYLAMINE ON THE FLUORESCENCE PROPERTIES OF 3-AMINOBENZOIC ACID *Sanjay Pant, Shahid Husain, Nisha Fatmaa, Nupur Pandeya and Mohan Singh Mehata*
PC-48	OCTUPOLAR CYCLOTRIPHOSPHAZENE-CORED SELF-STANDING COVALENT ORGANIC FRAMEWORK MEMBRANES AS NONLINEAR OPTICAL MATERIALS: IMPACT OF LINKAGE TYPES AND MATERIAL FORMS *Suresh Bommakanti,Satyapriya Nath, Rudrashish Panda, Sankalpa N. Panda, Ritwick Das and Bishnu P. Biswal*
PC-49	CHIRAL SELECTIVE SELF-ASSEMBLY OF NANOCELLULOSE CHIRAL C-DOT FILM SUPERIOR PLATFORM FOR CHIRAL SENSING *Sapna Waghmare and S. Mondal*
PC-50	EXPLORING MOLECULAR CHIRALITY THROUGH VIBRATIONAL CIRCULAR DICHROISM (VCD): A NEW FRONTIER IN SPECTROSCOPY *Saiprakash Rout and Himansu Sekhar Biswal*
PC-51	UNRAVELING LIPID DROPLET DYNAMICS DURING FERROPTOSIS USING A NOVEL D-A-D FLUORESCENT PROBE *Shrishti P. Pandey, Arkaprava Chowdhury and Anindya Datta*
PC-52	SUSTAINABLE PHOTOCATALYSIS BY EARTH-ABUNDANT OUTER AND INNER TRANSITION METALS *Ravi Kumar Venkatraman, Deborin Ghosh, Theis I. Sølling, Andrew J. Orr-Ewing and Ahmed M. El-Zohry*

PC-53	SYNTHESIS AND FUNCTIONALIZATION OF EXTENDED π CONJUGATED FLUORESCENT DYES FOR TARGETED ORGANELLE IMAGING *Simran and Sriram Kanvah*
PC-54	SOLVENT-DRIVEN PHOTOPHYSICS AND COMPUTATIONAL STUDY OF AN AMINOQUINOLINE DERIVATIVE *Nupur Pandey, Sanjay Pant, Nisha Fatma and M.S. Mehata*
PC-55	FLUORESCENT BASED HYDRAZIDE SCHIFF BASE FOR SELECTIVE DETECTION OF ANTIBIOTIC RESIDUES IN FOOD SAMPLES *P. Jeba Sagana and K. Swarnalatha*
PC-56	SARS CoV-2 FUSION PEPTIDE PROMOTES HEMIFUSION FORMATION IN ACHOLESTEROL-DEPENDENT FASHION *Priyanka Mahapatra, Smruti Mishra and Hirak Chakraborty*
PC-57	SULFATION OF HYALURONIC ACID RECONFIGURES THE MECHANISTIC PATHWAY OF BONE MORPHOGENETIC PROTEIN-2 AGGREGATION *Priyanka Panigrahi, Devi Prasanna Behera, Suchismita Subadini and Harekrushna Sahoo*
PC-58	NAPHTHALIMIDE: A NOVEL ESPT-DRIVEN PHOTOREMOVABLE PROTECTING GROUP FOR CONTROLLED RELEASE OF ALCOHOLS *Suchhanda Biswas and N. D. Pradeep Singh*
PC-59	AGGREGATION INDUCED EMISSION ENHANCEMENT BASED FLUORESCENT PROBE FOR THE DETECTION OF HYPOCHLORITE ION *Abinaya Muthukumar and K. Swarnalatha*
PC-60	SYNTHESIS, CHARACTERIZATION AND PHOTOPHYSICAL STUDIES ON LEAD-FREE INDIUM DOPED SILVER-BISMUTH-BASED DOUBLE HALIDE PEROVSKITE NANOCRYSTALS *Sumit Kumar Pradhan and Moloy Sarkar*
PC-61	ARTIFICIAL LIGHT HARVESTING SYSTEM BASED ON CASCADE FRET IN DNA TEMPLATED MULTICHROMOPHORIC SUPRAMOLECULAR ASSEMBLIES *Supratim Koley, N. Barooah, J. Mohanty and A. C. Bhasikuttan*

PC-62	ELUCIDATING THE ROLE OF SOLVENT ON THERMALLY-ACTIVATED DELAYED FLUORESCENCE *Sushree Suhani Puhan and Palas Roy*
PC-63	THE ULTRA-SMALL METAL NANOPARTICLES SUPPORTED ON N-DOPED CARBON FOR PHOTO-CATALYTIC DEGRADATION ORGANIC DYES AND NITROPHENOL REDUCTION *Supriya Panda, Biplab Kumar Manna and Sudip Barman*
PC-64	GAS-PHASE NUCLEOPHLIC ABSTRACTION OF HYDROGEN BY OZONE IN SATURATED HETEROCYCLES *Anmol Virmani, A. Saha, M. P. Walavalkar, A. Sharma, S. Sengupta and A. Kumar*
PC-65	Mg^{2+}-DOPING INDUCED MODULATION OF ULTRAFAST EXCITON DYNAMICS IN $FAPbBr_3$ NANOCRYSTALS *Tapas Pal, Prajit Kumar Singha, Ankit Kumar and Anindya Datta*
PC-66	ULTRAFAST INSIGHTS FULL-COLOUR LIGHT-EMITTING C-DOTS TO REVEAL THE CORE AND SURFACE STATE HETEROGENEITY DURING ELECTRON TRANSFER *Umarfaruk S. Sayyad and Somen Mondal*
PC-67	PYRANO[3,2-C] CHROMENE BASED SENSOR FOR DETECTION OF MICROBIAL AND HUMAN CONTAMINATION IN ENVIRONMENTAL SAMPLES *Vidhyashree M. and John Prakash*
PC-68	CHARGE CARRIERS DYNAMICS IN $CsPbBr_3$-PbSe EPITAXIAL NANOCRYSTAL HETEROSTRUCTURES *Rakesh Kumar Behera and Hirendra Nath Ghosh*
PC-69	SYNTHESIS OF 4-AMINOPHTHALIMIDE (4-AP) DERIVATIVES AND ITS PHOTOPHYSICAL PROPERTIES *Subiksha Asokan, Arulmozhi Puhazhendi, Pavan Kumar Mandali and Soumya Sivalingam*
PC-70	SYNTHESIS AND CHARACTERIZATION OF TYROSINE STABILIZED SILVER NANOCLUSTERS AND ITS ANTICANCER ACTIVITY *Apeksha Jagdale, Geeta K. Sharma, Santosh Terdale, Smriti Mittal, Ganesh Bose and Beena G. Singh*

PC-71	EFFICIENCY OF ENCAPSULATION OF THIOFLAVIN T (ThT) INTO DIFFERENT BILE SALT AGGREGATES: A FEMTOSECOND FLUORESCENCE STUDY *Ritwik Hazra and N. Sarkar*
PC-72	PHOTOCATALYTIC REACTION OF L-TYROSINE IN THE PRESENCE OF COLLOIDAL CdS *Pratigya Rizal and Devendra P. S. Negi*
PC-73	STUDIES OF PHOTOPHYSICAL BEHAVIOR OF FLUORESCENT CATIONIC DYE IN CUBOSOMES: THEIR USE IN SENSING APPLICATIONS *Kedar R. Khaparkhuntikar, A. Chatterjee and M. Banerjee*
PC-74	DESIGNING OF FOUR SYSTEM FRET SERIES & ITS APPLICATIONS *Jaiyanth Somasundaram and John Prakash*
PC-75	DESIGN AND APPLICATION OF FLUORESCENT PURINE PROBE FOR ER IMAGING AND STRESS MONITORING *Gayatri Bhattad, Anant Kapdi and Sriram Kanvah*
PC-76	ULTRAFAST ENERGY TRANSFER AND ELECTRON TRANSFER DYNAMICS IN TETRARYLPYRROLO[3,2-*b*] PYRROLE-BODIPY DYADS *Bipasha Dehariya, Richa Agrawal, Soumyaditya Mula and Rajib Ghosh*
PC-77	ULTRAFAST ANTI-AROMATICITY RELAXATION DYNAMICS IN p-DIACETYLPHENYLENEDIAMINE - A SMALLEST RED LIGHT EMITTER *Ankita Mutsuddi, Aruna K. Mora, Mrunesh Koli, Soumyaditya Mula and Sukhendu Nath*

Invited Talks (IT)

IT - 1

RADIATION INDUCED SYNTHESIS AND MODIFICATION OF MATERIALS

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Search for long-lasting products with better functionality and synthesized through energy efficient routes has been human endeavor since time immemorial. In pursuit of this use of ionizing radiation for material synthesis and modification has ushered an era of radiation processed products for wide spectrum of applications. The ability of ionizing radiation to initiate chemical reactions at room and sub-room temperatures that too without any additives has established ionizing radiation as a unique tool particularly for heat sensitive materials and where ultra-clean products are desired.

BARC with one of its mandate to develop non-power applications of nuclear technology has extensively worked on high energy gamma and electron beam (EB) irradiation effect on several materials of interest to sectors like industry, healthcare, agriculture and environment and developed in-house R&D capabilities as well as pursuing joint R&D work with leading institutes and industries [1]. Irradiation of polymers for generating crosslinked structure, or decrease molecular weight or for combining properties of two diverse polymers has been extensively investigated. Crosslinking of polymers in presence of suitable fillers results in flexible composites with radiation attenuation capability or electro-conducting composites suitable for analyte and strain sensing [2]. Radiolysis of water generates strong oxidising and reducing species. Thus, radiolysis of aqueous solution of pollutants under conducive conditions with understanding of underlying radiation chemistry can be exploited to mineralize recalcitrant pollutants. Radiation sterilization of medical products has long been established and can be extended to generate non-pathogenic organic manure from sewage sludge considered a waste. Utilization of radiation processed sewage sludge a rich source of organic carbon and micro-and macronutrients would be an economic way to improve soil health, and make full use of potential of sewage sludge [3]. Ionizing radiation can cause defects even in diamond matrix. Depending on the types of defects and trapped impurities irradiated diamond develop different colours which adds to the value of otherwise low-cost diamond pieces generated during cutting and polishing.

The talk will present an overview of different activities related to radiation processing of materials. Fundamentals of the radiation interaction with matter will be touched upon. Some unique benefits of using radiation as a tool for material processing, underlying principles and mechanisms of radiation-induced changes in the materials will be discussed.

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IT - 2

STIMULI-RESPONSIVE MOLECULAR ASSEMBLIES FOR THERANOSTIC APPLICATIONS

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Recent focus has been on designing molecules, molecular assemblies or molecular composites that can deliver therapeutically active molecules or reactive species to the disease site. However, challenges lie in maintaining the desired therapeutic efficacy, site specificity and minimal systemic cytotoxicity towards human physiology [1].Very recently, attempts have been made to address this complex issue using purpose-built stimuli-responsive therapeutics. Advances in utilising the optoelectronic properties of purpose-built molecular assemblies have contributed significantly to designing various stimuli-responsive drug delivery systems to improve drug efficacies. Some of our recent efforts to demonstrate the proof-of-concept of designing appropriate prodrug or molecular composites for treating cancer or certain bacterial stains will be discussed [2,3].

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IT - 3

RADIATION CHEMISTRY: AN UNEQUIVOCAL TOOL FOR STUDYING FREE RADICAL REACTION

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The genesis of radiation chemistry begins form the interaction of material with ionizing radiations in the MeV energy range. At the molecular level, these interactions open up very exciting chemistry that attracts researchers for solving various chemical phenomena. Due to large amount of energy deposition by the ionising radiation, a wide variety of transient species in the form of ions and radicals are produced. By maintaining suitable reaction condition, it is possible to selectively produce particular radicals and study their reactions. With the advent of high energy particle accelerators with real time detection systems one can follow the transients' spectral and temporal behaviour. In BARC, we use steady state (Co-60 gamma irradiation facility) and time resolved (LINAC based pulse radiolysis setup) to study the reactions of radiolytically generated radicals with different molecules to understand the site of radical attack, spectral behaviour of the transient and kinetic information. In a few occasion product identifications for the radical reaction are also possible by using different analytical techniques. In this talk, oxygen, sulfur and selenium-based compounds were used to study the reaction with hydroxyl radical and other radicals.

IT - 4

IONIZATION OF MOLECULES AND CLUSTERS UNDER INFLUENCE OF LASER AND ELECTRIC-DISCHARGE PULSE

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Gas-phase clusters are defined as weakly bound aggregates of atoms and molecules. Upon excitation, these clusters exhibit diverse reactions, which are distinct from those exhibited by their isolated constituent monomer units. Such distinct behaviour exhibited by clusters can be ascribed to close proximity of atomic/molecular species, coupled with existence of strong intramolecular bonds and weak intermolecular forces within the cluster.

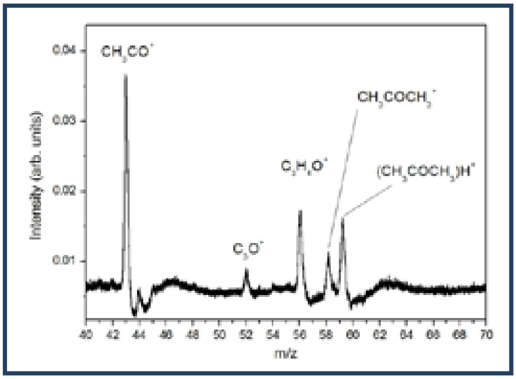

Figure 1. Time-of-flight mass spectrum obtained upon pulsed discharge ionization of acetone seeded in inert carrier gas

Our work is directed towards understanding behaviour of these clusters under influence of intense laser pulses and pulsed electric discharge. Upon interaction with intense laser, clusters exhibit unusual photochemical behaviour resulting in generation of exotic molecular species, multiply charged energetic atomic ions, energetic electrons and high energy photons. Such characteristic behaviour of clusters has been ascribed to intrinsic properties of clusters i.e. finite size, solid-like number density, their secluded existence in gas-phase and cooperative behaviour of cluster constituents under the influence of intense laser pulse.Extensive studies carried out by our group emphasises on factors which influence efficient transformation of laser energy upon interaction with clusters into particle energy i.e. energetic multiply charged atomic ions and electrons [1]. Besides studies have also been carried out on organic molecules and clusters subjected to electric pulse discharge. These studies are of relevance for plasma pyrolysis of volatile organic compounds and laboratory astrochemical investigations. For studies carried out on acetone, under pulsed discharge conditions (Figure 1), endoergic reactions involving stepwise dehydrogenation of acetone was found to be a predominant channel leading to formation of $C_3H_4O^+$ and C_3O^+ ions [2]. In the presentation, some of these experimental findings will be discussed with emphasis on mechanism, which leads to generation of unusual atomic and molecular species under the influence of laser and pulse electric discharge.

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IT - 5

ULTRAFAST DYNAMICS OF SINGLET FISSION: MECHANISTIC INSIGHTS FROM FEMTOSECOND AND NANOSECOND TRANSIENT ABSORPTION SPECTROSCOPY

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Singlet fission (SF), a spin allowed process in organic materials splits singlet exciton into a pair of triplets which can potentially improve photovoltaic efficiency beyond Shockley-Quisser limit[1]. However, due to energetic and kinetic constraints, SF is restricted to only a few select class of organic molecules. Optimization of SF process requires balance of several molecular parameters and hence need detailed mechanistic understanding of the process. Spectroscopic assessment of SF kinetics and establishing structure-dynamics relation is imperative to optimize SF yield in existing and new organic materials. Merit of SF mechanism for exciton doubling in several polyacene based organic semiconductor materials were evaluated by ultrafast spectroscopic measurements[2-5]. Inducing strong intermolecular coupling by close π-π interaction and long range crystalline order is revealed to be important criteria for efficient SF which has been exemplified by comparing ultrafast dynamics of different polyacene derivatives (namely, phenylethynyl (BPEA) vs triisopropylsilyl (TIPSAn) derivatives of anthracene). Bulky triisopropyl group in TIPSAn is shown to decrease intermolecular coupling reducing singlet fission process, as opposed to efficient SF (>90%) in planar BPEA derivative. Importance of crystalline order and sample morphology on SF kinetics for long lived triplet generation is shown in BPEA nanoaggregates of different size. Mechanistic insight on the role of charge transfer state as an intermediate in SF process is obtained in diketopyrrolopyrrole derivatives, where ultrafast population of CT state followed by triplet pair generation is resolved in picosecond timescale. Importance of structural and morphological tuning of SF dynamics and potential scope of utilization of these materials in photovoltaic devices will be discussed.

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IT - 6

SEQUENCE OF PROTEIN ALPHABETS PRESCRIBES THE SECONDARY STRUCTURES OF PEPTIDES: A COMPREHENSIVE PICTURE FROM CONDENSED AND GAS PHASE STUDIES

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Secondary structures of peptides and proteins are dictated by the hydrogen bonding interactions in the backbone as well as the sequence of the amino acid residues present there. In general, secondary structures of the peptides and proteins are stabilized by α-helix, β-sheets and several types of turns namely C7 (γ-turn), C10 (β-turn), and C13 (α-turn) hydrogen-bonded rings formed through inter-residue interactions in the backbone. Being local in nature, the secondary structures of the peptides can be probed by investigating small capped peptides, which represent these interactions in larger peptides and proteins. Out of the 20 amino acids, glycine (Gly) and proline (Pro) are quite unique because there is no side chain in the former one, while the side chain of the latter one is connected with the nitrogen atom to form a five-membered ring. Thus, the most flexible amino acid, Gly, and the most rigid amino acid, Pro are found very often in the loop region of the β-hairpin structures of the proteins. Interestingly, it has been found that the -Pro-Gly- sequence has a higher propensity for the formation of the β-turn conformation while the -Gly-Pro-sequence prefers to form an extended polyproline II type conformation. It is also known that the β-turn conformation is the requirement of the enzymatic hydroxylation of the specific proline residue of the -Pro-Gly- segment in procollagen for the formation of a stable triple helical structure of collagen. In this talk, I will be presenting a comprehensive overview of the folding motifs of several Pro-Gly containing peptidesthrough FTIR, 2D-NMR, gas phase laser spectroscopy, single crystal XRD, and quantum chemistry studies. The results exhibit a fine interplay of the intrinsic conformational properties, crystal packing and solvation of the peptides. A detailed understanding of the motifs of the secondary structures of the peptides can help in engineering these exotic non-covalent interactions in designing improved therapeutic peptides, supramolecular assemblies etc.

IT - 7

OXIDATION UNVEILED: BRIDGING ATMOSPHERIC CHEMISTRY AND HUMAN PHYSIOLOGY

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Oxidation processes play a crucial role in both atmospheric chemistry and human physiology, serving as fundamental mechanisms that drive various biochemical and environmental transformations. In the atmosphere, oxidation reactions are essential for the degradation of pollutants, the formation of secondary organic aerosols, and the regulation of greenhouse gases, thereby influencing climate and air quality. Similarly, in the human body, oxidation processes are integral to metabolic pathways, including cellular respiration and the detoxification of harmful substances. Both systems rely on the transfer of electrons, highlighting a fundamental similarity in their underlying chemical principles. Furthermore, while atmospheric oxidation contributes to the balance of ecosystems and the maintenance of environmental health, biological oxidation processes are vital for energy production and the maintenance of homeostasis. Understanding these processes and their interconnections underscores the importance of oxidation in sustaining life and the environment, emphasizing the need for continued research into their mechanisms and impacts. This dual perspective fosters a holistic appreciation of oxidation as a pivotal element in both ecological and physiological contexts.

IT - 8

PORPHYRINS & ITS ANALOGUES:APPLICATION AS A CHEMOSENSOR

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Calixphyrins are structural hybrids of porphyrins and calixpyrroles. The pyrrole units in the macrocyclic core are bridged by sp^2 and sp^3 hybridized *meso*-carbon atoms. This leads to partial interruption in the conjugation pathway of the macrocycle, introduces novel structural features, thus leads to stabilization of anion and cation in the core. In the first part of my talk, we will focus on synthesis of arene ring incorporated expanded calixphyrins and explores, in particular, (i) Calix-*m*-benzophyrin with AIEE characteristics and application as a Hg(II) chemosensor[1]; (ii) strapped calixphyrins as Fe(III) sensor; (iii) higher analogue of calix-*m*-benzophyrin and its vapoluminescent response with volatile organic compounds, and(iv) Chemodosimetric cyanide sensing of 5,15-porphodimethene Pd(II) complex [2].

On the other hand, porphryins are conjugated aromatic macrocycles and effectively utilized as materials, medicine and catalysis. In the second part of my talk, we will highlight the synthesis of arene or pyridyl ring incorporated contracted porphyrinoids and explores, in particular, (i) Bipyricorrole: A corrole homologue and its fluorescence Zn(II) sensor,[3] and (ii) Dicarbatriphyrin (2.1.1) and its selective sensing with Fe(III) ions [4]. Overall, in this lecture, we mainly focus sensing properties of expanded calixphyrins and contracted porphyrins.

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IT- 9

MACROCYCLIC HOST-BASED FUNCTIONAL SUPRAMOLECULAR ASSEMBLIES: APPLICATIONS IN CATALYSIS, SEPARATION, AND THERAPEUTICS

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Research on supramolecular assemblies of organic/inorganic guests using various macrocyclic receptors and biomolecules is growing rapidly as they provide a unique way to control the sophisticated nano-architectures to create supramolecular functional assemblies. Among many different strategies for making such functional assemblies, non-covalent host-guest interactions have recently received great attentions in a variety of scientific fields due to their unique assembly characteristics, functional performances and potential applications in catalysis, fluorescent sensors, drug delivery, adsorbents, etc. Macrocyclic hosts such as cucurbiturils (CBs), calixarenes (CXs) and cyclodextrin (CD) derivatives have gained immense research interest because of their ability to host, in a highly selective manner, certain types of guest molecules such as metal cations, polyoxometalates, boron-based hydride along with the protonated alkyl and aryl amines, cationic dyes and drugs through ion-dipole interaction and hydrophobic interactions. This presentation will cover our recent work on the macrocyclic host-assisted functional materials of few organic/inorganic guests having technological and biological importance and their projected applications toward the H_2 generation, white LED fabrication, ^{99m}Tc radionuclide separation, amyloid fibril inhibitors and antibacterial agents.

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IT - 10

REDOX-ACTIVABLE HEAVY ATOM FREE PHOTODYNAMIC THERAPY

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Photodynamic therapy (PDT) has emerged as a powerful tool to treat skin cancer and other diseases. In PDT, a photosensitizer (PS) is used to produce different reactive oxygen species (ROS) upon photoirradiation, which causes cell death. However, in most cases, the PS consists of metals or heavy-atoms with significant cytotoxicity, even in the dark. Thus, in the recent past heavy atom free organic photosensitizers have gained significant attention. We envisaged the scope and utility of the therapy would be enhanced if such organic PS can be delivered in a dormant state and activated selectively by a biological stimulus, because it provides a secondary shielding if the PS becomes active by a specific biological stimulus, rather than just manual light activation. With this broad objective, we have explored PDT using the thionated naphthalene-monoimide based newly synthesized hydrophobic PS (NMI-S), which showed excellent ROS generation ability. For delivery purpose, it was non-covalently sequestered in a redox-responsive amphiphilic ABA-type block copolymer micelle in which the hydrophobic B block consists of bio-reducible polydisulfides chain. within a redox-responsive polymer. This encapsulation initially reduces the generation of ROS as the PS remains in the aggregated state by antiparallel stacking inside the hydrophobic confined environment of the polymersome. However, when exposed to glutathione (GSH), a tripeptide commonly overexpressed in cancer cells, the polymer disassembles, releasing NMI-S in its active form, which effectively kills over 70% of cancer cells upon photoirradiation [1]. After evaluating the efficiency of the encapsulated PS, another redox responsive polymer with conjugated PS was designed with an objective to investigate the possibility of further improvement by cascade degradation of the polymeric backbone to release the active PS. The PS was covalently conjugated with a poly-disulfide backbone by carbonate linker (P1). P1 showed spontaneous self-assembly in water, due to its amphiphilic nature, and produced nanoparticles (~ 150 nm). In such nanoparticle, the PS is expected to remain aggregated in the core, which resulted in deactivation of its ROS generation ability, which is consistent with our earlier results. In presence of glutathione (GSH), it showed disassembly resulting in reactivation of the ROS generation ability. Mass spectrometry supported the cascade degradation mechanism, as the anticipated products could be clearly identified. P1 showed excellent cellular uptake and light-triggered highly efficient cell killing (> 90 %). This presentation will show highlight of these recent results from our group.

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IT - 11

UNLOCKING THE POTENTIAL OF 10,12-PENTACOSADIYNOIC ACIDS AS MULTIFUNCTIONAL DUAL-OUTPUT CHEMOSENSORS

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10,12-Pentacosadiynoic acid (PCDA) has emerged as a promising platform for designing multipurpose dual-output chemosensors. Known for its unique polymerization and chromatic properties, PCDA can respond to various analytes with both colorimetric and fluorometric outputs, providing a versatile tool for rapid and sensitive detection. This dual-output capability arises from the acid's conjugated polymer backbone, which undergoes structural and electronic changes upon interaction with target analytes, leading to distinct visual and fluorescent signals. The dual-sensing nature of PCDA-based chemosensors makes them ideal for applications in environmental monitoring, biomedical diagnostics, and chemical safety, where rapid and reliable detection of analytes is critical. This talk will covers the use of PCDA in chemosensing applications, highlighting its adaptability, sensitivity, and potential for integration into portable detection systems.

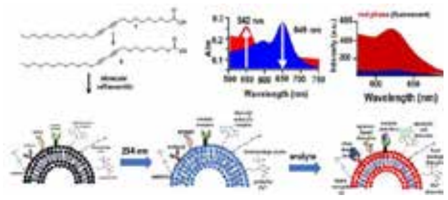

Figure 1. Schematic representation of sensing mechanism of polydiacetylene-based sensors.

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IT - 12

RADIATION INDUCED SYNTHESIS OF POLYMERIC SYSTEMS FOR VARIOUS BIOMEDICAL APPLICATIONS

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High energy radiation in the form of gamma rays, X-rays, electron beams, ion beams etc can be used as a tool for synthesis of polymers in various forms including hydrogels, nanogels, nanofibres etc. Irradiation of aqueous solution of polymers leads to formation of very reactive intermediates in the forms of excited states, ions and free radicals. These intermediates take part in various reaction pathways leading to formation of new bonds and structures. The ultimate effects of these reactions are the formation of oxidized products, grafts, crosslinking and scissioning of main or side chains. The relative extend of these transformations depend on the nature of the polymer, conditions of treatment before, during and after irradiation and close control of these factors make the modification of polymers possible by radiation processing.

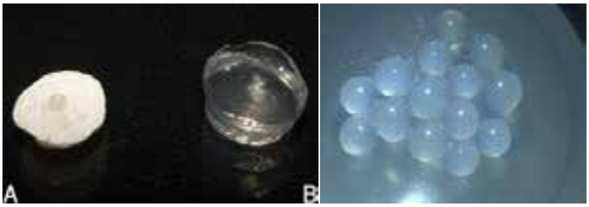

Figure 1. Glycopolymeric hydrogel and microspheres synthesized by gamma radiation induced polymerization.

The talk will cover different systems including synthetic polymers and natural polymers subjected to gamma radiation induced crosslinking to form polymeric hydrogels. Radiation degrading type natural polymers can be converted to hydrogels by incorporating radiation crosslinking type polymers into the matrix in suitable proportions. Gamma radiation induced synthesis of PVA-gum acacia hydrogels with insitu formed silver nanoparticles were studied for wound dressing applications[1]. A new class of biocompatible and biodegradable materials containing sugar moieties called as glycopolymers have received great attention in the scientific community[2]. This is largely due to their wide range of applications, which include, the synthesis of macromolecular drugs, matrices for cell culture, model biological systems, surface modifiers, chromatographic purposes and so on. The advanced polymerization techniques have facilitated the synthesis of glycopolymers of different types required for specific applications. Glucose, mannose and galactose-based polyacrylamides were synthesized from the corresponding monomers by gamma irradiation. The radiation polymerized glycopolymers exhibited pH dependent self-assembly behaviour in solution.

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IT - 13

SINGLE MOLECULE SPECTROSCOPY OF EMERGING NANOMATERIALS FOR SUPER RESOLUTION OPTICAL IMAGING

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Single molecule spectroscopy and microscopy (SMSM) have revolutionized to unveil various hidden and complex properties of molecules and materials that was not possible using the bulk measurement. By removing the ensemble averaging of thousands of molecules in bulk system, SMSM allows to study the photophysics and photochemistry at a time and explore the hidden heterogeneity in complex condensed phases. In recent years, several classes of nanomaterials are emerging for their various applicationswhere the photoluminescence of these materials plays significant role. Understanding the exact mechanism of the photoluminescence of these nanomaterials often encounters number of challenges. Our group mainly focusing on understanding the photophysical aspects of these nanomaterials at single molecule level. I will present some of the recent development in unveiling the state-of-art optical mechanism of some of the emerging nanomaterials like carbon nanodots, coinage metal nanoclusters and metal complexes. I will, further, discuss how this information is carry forwarded for their vast applications in Stochastic Optical Reconstruction Microscopy (STORM) and Super Resolution Radial Fluctuation Microscopy (SRRF) for cellular organellar dynamics by breaking the fundamental laws of light diffraction.

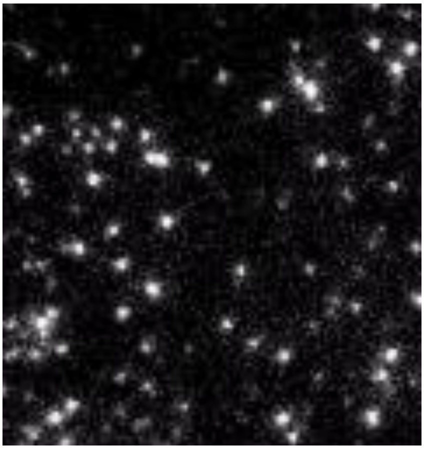

Figure 1. Single molecule image of fluorescent nanomaterial showing individual bright spots.

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IT - 14

PHOTOPHYSICS OF HYBRID LIGHT-MATTER STATES

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Strong coupling achieved at room temperature using molecular systems enabled us to study the unusual behavior of half-photon, half-molecule hybrid states, called polaritonic states. These states show the delocalization of a cavity photon with a large number of molecular transitions. For example, one can easily tailor the photoluminescence of the polaritonic states by fine-tuning the photon-exciton mixing fractions in 2D materials.[1] We recently studied these systems in open cavities and generated clean data that are quantized in polarization, momentum, and energy.[2] Further, we used donor-acceptor pairs spatially separated and tested long-range energy transfer in the strongly coupled system.[3] Our experimental findings suggest the potential of strong light-matter coupling for use in quantum sensing and communication. During the talk, I will introduce the concept of strong coupling and its application in real systems.

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IT - 15

WATER-ENHANCED DES ELECTROLYTES FOR STABLE ZINC-ION BATTERIES

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Aqueous Zn-ion batteries (ZIBs) are emerging as safer and more sustainable alternatives to traditional Li-ion batteries. Among the critical components of ZIBs, the electrolyte plays a key role in determining electrochemical performance and battery efficiency. However, conventional aqueous electrolytes pose challenges for Zn anodes, including poor reversibility and limited cycling stability caused by dendrite formation. To address these issues, "Water-in-Deep Eutectic Solvent (DES)" electrolytes have garnered attention as eco-friendly and cost-effective solutions. Despite their promise, fundamental questions remain unanswered: the optimal water content in DES, the effect of water on electrolyte dynamics, the disruption of DES hydrogen bonding networks, and the changes in the Zn^{2+} solvation structure in water-in-DES systems.

Using ultrafast 2D IR and 2D NMR spectroscopy, we investigate solvent dynamics, structural rearrangements, and hydrogen bonding behavior across varying water concentrations, both with and without Zn salts. Complementing these experimental methods, molecular dynamics (MD) simulations provide insights at the molecular level. Our findings reveal that adding 10 moles of water per mole of DES optimizes electrolyte performance, as confirmed by peak conductivity in impedance spectroscopy. These results offer valuable insights into improving ZIB electrolytes and enhancing their practical applicability.

IT - 16

ROLE OF RADIATION CHEMISTRY IN NUCLEAR TECHNOLOGY & BEYOND

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Radiation chemistry, the study of chemical reactions initiated by ionizing radiation, plays a crucial role in various aspects of nuclear technology, starting from safe reactor operation, material degradation by corrosion due to the reactive species from the radiolysis of coolant and moderator, reprocessing and nuclear waste management. It provides fundamental insights into the behavior of materials and substances under radiation exposure, essential for ensuring efficiencyandsafety inoperating nuclear power plants and other nuclear facilities [1]. Emphasis on water radiolysis in the nuclear industry comes from the interaction of different types of radiation (alpha, beta, gamma or recoil nuclei with enough energy) to break the water (used as coolant and moderator) molecules in water-cooled nuclear reactors. In addition to understanding the interaction of radiation with water, it is important to consider the steady-state concentrations of radiolytic products like H_2 and H_2O_2formation. These parameters are essential in controlling corrosion rates of the water circuitries as the oxide solubility is pH-dependent. Any changes in water chemistry directly affect the radiolytic yields and the prevailing redox environment, affecting the nature and morphology of surface oxide films for their long-term reliability.

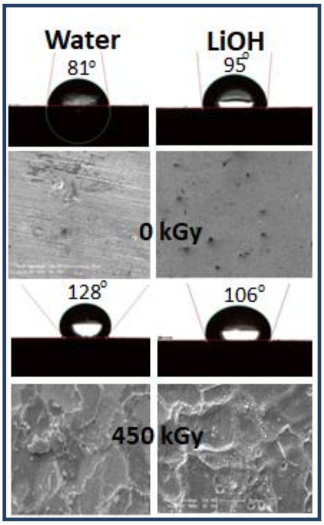

Figure 1. Surface morphology and contact angle of Carbon Steel in water and LiOH before and after irradiation.

Beyond nuclear technology, radiation chemistry plays a crucial role in biology and medicine for sterilization of medical devices, food products, as diagnostic and therapy.Ionizing radiation is used in pollution control by degrading organic pollutants such as pesticides and industrial effluents. A basic understanding of the radiation chemistry mechanism is used to develop a variety of innovative nanomaterials with controlled size, shape, and properties, enhancing their functionality and modification of the surface properties.

The talk will give a comprehensive picture of the basics in radiation chemistry, some selected technological issues related to water-cooled reactors and nano-oxide synthesis.

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IT - 17

STUDY OF GOLD NANOPARTICLES INTERACTION WITH N, N, N’ , N’ –TETRAMETHYL-p-PHENYLENEDIAMINE RADICAL CATION USING STEADY STATE RADIOLYSIS

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The interaction of gold nanoparticles with N,N,N′,N′-tetramethyl-p-phenylenediaminecation (TMPD$^{\bullet+}$), formed by the reaction of azidyl radical ($N_3^{\bullet}$) with N,N,N′,N′-tetramethyl-p-phenylenediamine in aqueous solution were investigated using steady state radiolysis. The build-up of TMPD$^{\bullet+}$ absorbance peak at 565 nm were monitored using UV-visible spectrophotometer at different irradiated dose from a ^{60}Co γ source with a dose rate of 4.16 Gy/min with and without gold nanoparticles (AuNPs). The variation of the yield in presence of AuNPs at lower and higher irradiation dose suggests complicated plausible electron transfer mechanism which will be highlighted in the talk. The study suggests a direction for investigation of interaction of free radicals with nanomaterials using the fundamentals of radiation chemistry.

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IT - 18

OPTIMIZING ION IRRADIATION TECHNIQUES TO SIMULATE NEUTRON-INDUCED DAMAGE IN NUCLEAR REACTOR CORE MATERIALS: INSIGHTS FROM VECC THROUGH EXPERIMENTAL AND SIMULATION STUDIES

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Ion irradiation studies have demonstrated their effectiveness in emulating the neutron-induced damage in nuclear reactors. By carefully controlling parameters such as dose, dose rate, and temperature, it is possible to simulate the equivalent damage experienced by core structural materials in reactor environments [1]. At the Variable Energy Cyclotron Centre (VECC), we have utilized various ion beams (light and heavy) over the past few decades to investigate the structure-property relationships in key candidate alloys for core component applications.

In this talk, we will present recent findings from our studies on vanadium alloys, a key candidate material for first-wall and blanket applications in fusion reactors [2], niobium alloys, which are being explored for compact high-temperature reactor applications [3] and pure Ni -the base material for the Ni based alloys for Molten Salt Breeder Reactor applications [4]. The resulting microstructural changes, as a function of dose after ion irradiation, were primarily characterized through detailed X-ray diffraction (XRD) line profile analysis further complemented by Transmission Electron Microscopy (TEM) and/or Positron Annihilation Spectroscopy (PAS) measurements. Mechanical property changes in the irradiated samples were measured to establish a correlation between the induced microstructural modifications and material performance. Furthermore, the resulting defect configurations were confirmed through successive cascade Molecular Dynamics (MD) simulations and ab-initio Density Functional Theory (DFT) calculations, enabling atomic-scale support of experimental observations and a deeper understanding of defect energetics, stability and configurations.

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IT - 19

FACET ENGINEER FORTAILORING PHOTOPHYSICAL PROCESSES IN PEROVSKITE NANOCRYSTALS

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Multi-faceted perovskite nanocrystals hold significant promise for advancing display and device technologies. Recently, the Pradhan group synthesized $CsPbBr_3$ perovskite nanocrystals (PNCs) with unconventional morphologies, including 12-faceted dodecahedrons and 26-faceted rhombicuboctahedrons[1]. Following their synthesis, Ghosh and colleagues demonstrated that the cooling of hot carriers in extra-faceted PNCs is polaron-mediated, resulting in slower carrier dynamics in extra-faceted PNCs[2]. Our research group, employing a femtosecond upconversion setup, revealed that hot carrier cooling in 26-faceted rhombicuboctahedron PNCs is delayed by over tenfold compared to their cubic counterpart [3]. Moreover, extra-faceted PNC complexed with a charge scavenger molecule serves as a model composite, where charge carriers are effectively harvested before they relax to the band edge by dissipating their excess energies[4]. These findings collectively underscore the potential of extra-faceted PNCs in real applications. Successful extraction of hot carriers holds the promise of significantly exceeding the Shockley–Queisser (SQ) limiting value (~33%) in solar cell device efficiency. In this discourse, I shall delve into several intriguing results pertaining to these extra-faceted PNCs[3-5].

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IT - 20

SUSTAINABLE NANOMATERIALS FOR SOLAR TO CHEMICAL ENERGY CONVERSIONS THROUGH COMPLETE METAL FREE APPROACH

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Considering two major alarming problems of modern society, *i.e.*- a) global warming and b) gradual depletion of traditional fossil fuels, it is utmost necessary to shift towards the alternative energy resourses. In this regard, photocatalytic H_2 evolution from water is considered one of the cleanest approach till date. H_2 is the cleanest fuel and does not produce any greenhouse gas upon direct combustion, or even while acting as a chemical feedstock for other transportable fuel generation. Therefore, it is highly desirable to produce efficient photocatalysts. Till date several advancements have been made with metal-based inorganic semiconductors. However, their practical applicability is still under debate considering the environmental sustainability, stability and economical expenses. As a result, it is essential to develop alternate photocatalysts that are environmentally sustainable, cost-effective, stable and highly efficient. The metal-free approach is one of the most promising approaches in contrast to the traditional metal based photocatalysts. In this regard, our major focus is to develop and optimizecomplete metal free sustainable nanomaterials made of earth abundant elements (*i.e.*- C, S, P *etc*) for solar H_2 production and simultaneous chemical energy conversions through optimizinglight-matter interactions and the desired photochemical processes for photocatalysis ranging from *ms* to *fs* time domain.

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IT - 21

DESIGN OF INTRINSIC WHITE LIGHT EMITTING PHOSPHORS AND THEIR W-LEDS

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Ever since the discovery of blue light-emitting diodes, a new era for white light-emitting diode (W-LED) phosphors has emerged. W-LEDs are typically produced by integrating a GaN blue diode with a YAG:Ce^{3+} yellow phosphor layer. However, these W-LEDs are unable to simultaneously achieve superior color rendering and stability. They also suffer from issues such as a bluish tinge (which can be harmful to the human eye retina), self-absorption, reduction in intensity, complex manufacturing processes, and degradation of various components.[1] The high color rendering index (CRI) of these LEDs often comes at the expense of luminous efficacy (LE). This trade-off is commonly observed in broad emission sources due to the absence of the red spectral region, leading to efficacy loss and low CRI.

The design of self-activated single-phase phosphors that can emit white light can address these issues by eliminating the need for multiple phosphors. Such self-activated phosphor can give rise to emission spanning over the entire visible region. This approach can offer improved balanced white emission with higher CRI, high LE, simple fabrication process, low cost (devoid ofmulti-phosphor cost), excellent color stability, and avoid any self-absorption or blue tinge. [2,3] The presentation will focus on the comprehensive findings related to the newly developed intrinsically balanced white light-emitting phosphors, which demonstrate improved color balance, a high CRI, and the mechanisms that facilitate red emission, eventually contributing to the generation of white light.

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IT - 22

CHIRAL LIGHT EMITTING NANOMATERIALS: FROM FUNDEMENTALS TO APPLICATIONS

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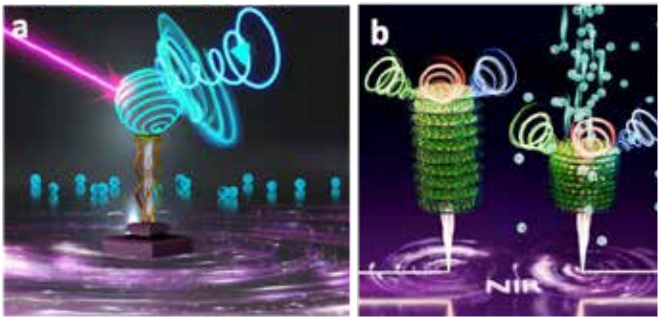

Figure 1. (a) Scheme illustrating circularly polarized luminescence in (a) downconversion and (b) upconversion luminescent nanophosphors.

Thewide application of chiral molecules in pharmaceuticalsand catalysis has trigerred extensive investigations on optically active systems using circular dichroism (CD) spectroscopy as the major tool. Observation of chirality in nanomaterials has rejuvenated the field and has captivated research interest in recent years[1]. Optical activity in nanomaterials can be achieved through: (i) the synthesis of intrinsically chiral nanoparticles, (ii) chiral induction using chiral ligands, and (iii) template assisted methods. Of late, research interest has focussed attention on chiral light emitting molecules and materials due to their their vast application in field of display devices, data encryption, chiral biosensing and bioimaging. Our recent attempts on the synthesis of chiral emissive nanomaterials, and the investigations on their excited state optical activity througugh circularly polarized luminescence (CPL) will be discussed. Unlike CD, CPL is a relatively new technique that has gained tremendous attention duto itscapability to probe the excited state charity. Working in this direction, we have recently demonstrated downconversion as well as upconversion CPL in different class of nanomaterials. Ligand induced downconversion CPL in metal clusters and template assisted upconversion CPL in lanthanide-based nanophosphors will form the topic of discussion[2,3]. Our recent attempts towards understanding the fundamentals of optical activity in nanomaterials and their potential applications in various fields will form the basis of the talk.

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IT - 23

Zn (II) COORDINATED SELF-ASSEMBLED DIPEPTIDE BASED FLUORESCENT NANOPARTICLES FACILIATE CELLULAR IMAGING AND TARGATED DRUG DELIVERY

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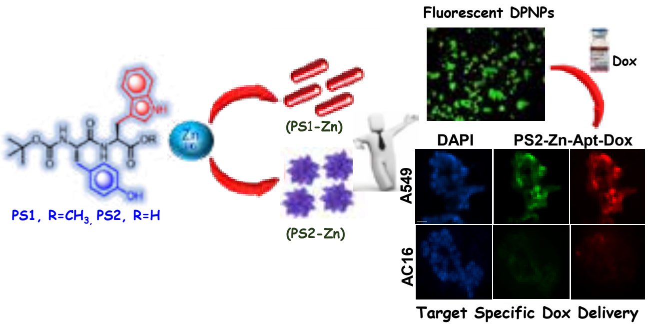
Self-assembled peptide-based nanostructures, comprised of naturally occurring amino acids, display excellent biocompatibility, biodegradability, flexible responsiveness, and synthetic feasibility and can be customized for several biomedical applications. However, the lack of inherent optical properties of peptide-based nanoparticles is a limitation in their use as imaging probes or drug delivery vehicles. To overcome this impediment, we generated Boc protected tyrosine-tryptophan dipeptide-based nanoparticles (DPNPs) with structure rigidification by Zn (II), which shifted the peptide's intrinsic fluorescent properties from the ultraviolet to the visible range. These DPNPs are photostable, biocompatible and have visible fluorescence signals that allow for real time monitoring of their entry into cells. We further show that two DPNPs (**PS1-Zn** and **PS2-Zn**) can encapsulate the chemotherapeutic drug doxorubicin (Dox) and facilitate intracellular drug delivery resulting in cancer cell killing actions comparable to the unencapsulated drug. Finally, we chemically modified our DPNPs with an aptamer directed toward the epithelial cell surface marker EPCAM, which improved Dox delivery to the lung cancer epithelial cell line A549. In contrast, the aptamer conjugated DPNPs failed to deliver Dox into the cardiomyocyte cell line AC16. Theoretically, this strategy could be employed *in vivo* to specifically deliver Dox to cancer cells while sparing the myocardium, a major source of dose-limiting adverse events in the clinic. Our work represents an important proof-of-concept exercise demonstrating that ultra-short peptide-based fluorescent nanostructures have great promise for the development of new imaging probes and targeted drug delivery vehicles



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IT - 24

Perturbation of Protein Conformation and Kinetics by Polyethylene glycol: A correlation between Ensemble and Single-Molecule approach

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The importance of macromolecules paves the way towards a detailed molecular level investigation as all most all cellular processes occurring at the interior of cells in the form of proteins, enzymes, and other biological molecules are significantly affected because of their crowding. Thus, exploring the role of crowding environment on the denaturation and renaturation kinetics of protein molecules is of great importance. Here, CRABP I (cellular retinoic acid binding protein I) is employed as a model protein along with different molecular weights of Polyethylene glycol (PEG) as molecular crowders. The experimental evaluations are done by accessing the protein secondary structure analysis using circular dichroism (CD) spectroscopy and unfolding kinetics using intrinsic fluorescence of CRABP I as well as extrinsic fluorophorescence at 37 °C to mimic the in vivo crowding environment. The unfolding kinetics results indicated that both PEG 2000 and PEG 4000 act as stabilizers by retarding the unfolding kinetic rates which is observed with both ensemble and single-molecule experiments. The molecular dynamics (MD) studies revealed that thirteen PEG 2000 molecules assembled during the 500 ns simulation, which increases the stability and percentage of β-sheet. The experimental findings are well supported by the molecular dynamics simulation results.

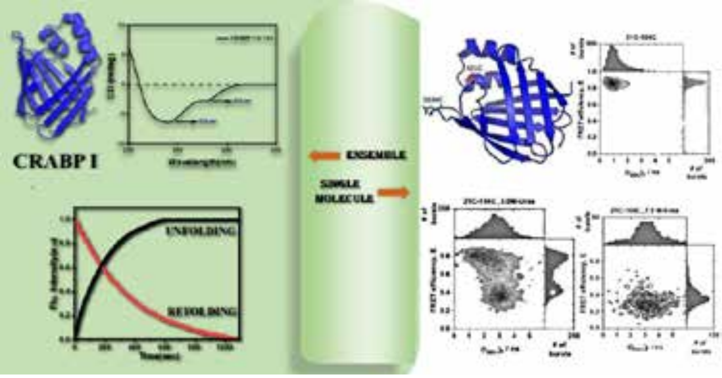

Figure 1. (Left) Depiction of CRABP I secondary structure and folding and unfolding kinetics & (Right) Distribution of native and non-native components during unfolding of CRABP I.

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IT - 25

MECHANISM OF MEMBRANE FUSION: INTERPLAY OF LIPID AND PEPTIDE

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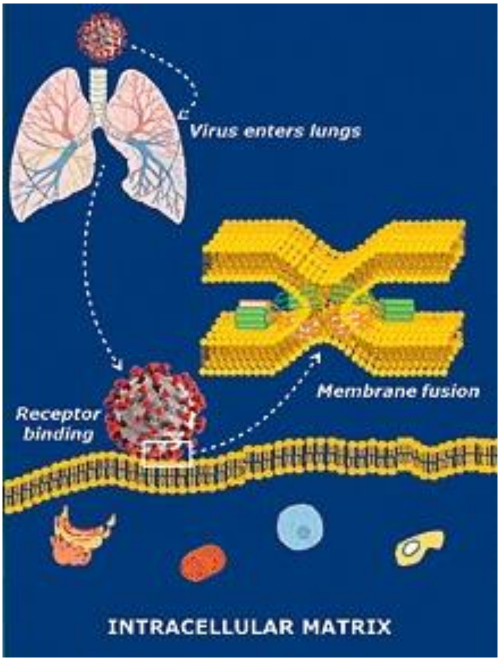

Membrane fusion is an essential process for the survival of eukaryotes and the entry of enveloped viruses into host cells. A proper understanding of the mechanism of membrane fusion would provide us with a handle to manipulate several biological pathways and design efficient vaccines against emerging and re-emerging viral infections. Although fusion proteins take the central stage in catalyzing the process, the role of lipid composition is also of paramount importance. Lipid composition modulates membrane organization and dynamics and impacts the lipid-protein/peptide interaction. Moreover, the intrinsic curvature of lipids has a strong impact on the formation of stalk and hemifusion diaphragm. Detection of transiently stable intermediates remains the bottleneck in the understanding of the fusion mechanism. To circumvent this challenge, analytical methods can be employed to determine the kinetic parameters from ensemble average measurements of observables, such as lipid mixing, content mixing, and content leakage. The current view aims to present an analytical method that would aid our understanding of the fusion mechanism, provide a better insight into the role of lipid shape, and discuss the interplay of lipid and peptide in membrane fusion.

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Short Talks (ST)

ST - 1

PSEUDOROTAXANE, METASTABLE ROTAXANE AND ROTAXANE-BASED MOLECULAR SWITCHES FOR ANION RESPONSIVE STUDIES

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Fluorescence active BP23C7 macrocycle forms anion-responsive pseudo[2]rotaxane with anthracene terminated axles. Due to the energy transfer at the excited state of pseudo[2]rotaxane, complete fluorescence quenching of BP23C7 was observed, which was recovered upon ion-pair formation with halide anions, leading to a "turn-on" sensing for halide anions, such as fluoride and chloride [1].To achieve selectivity in halide anion sensing, metastable [2]rotaxanes are constructed utilizing 23C7 macrocycle. The metastable [2]rotaxane comprising cyclohexyl end group undergoes deslippage of 23C7 in presence of fluoride anion, induced by ion-pair formation. However, the ion-pair strength with chloride, bromide and iodide anions are not strong enough for 23C7 macrocycle to surmount the steric barrier of cyclohexyl moiety, signifying the role of steric size of the end group. Fluoride anions, down to 2.4 x 10^{-7} M, could be detected by fluorescence turn-off of the anthracene band [2]. Next, in pursuit of achieving reversibility along with selectivity and sensitivity, bistable [2]rotaxane-based molecular switches are constructed using X23C7 macrocycles. Fluorescence turn-on could be observed as X23C7 underwent shuttling from ammonium site to the methyl triazolium moiety (MTA^+), selectively upon fluoride anion exposure, blocking the pathway for PET quenching of the anthracene moiety by MTA^+. The same can be followed by portable UV detector as well.

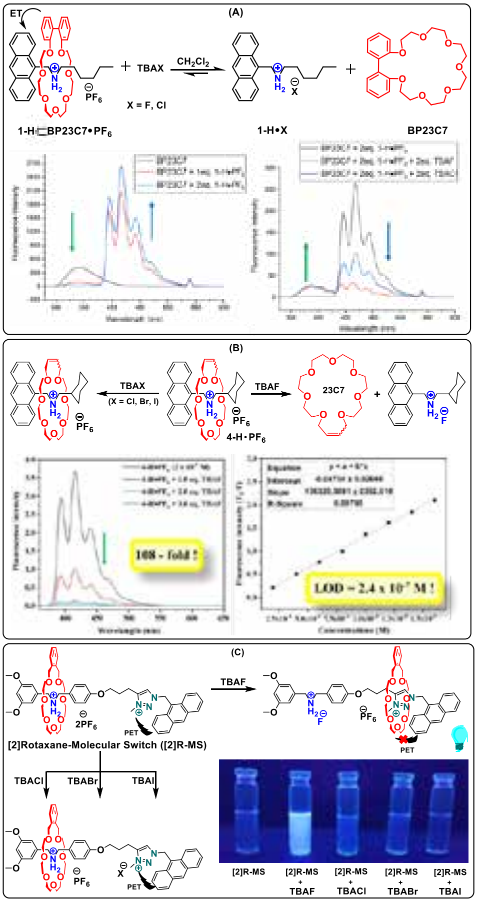

Figure 1. Spectrofluorimetric detection of halide anions using a) pseudo [2] rotaxane; b) metastable [2] rotaxane; c) [2] rotaxane molecular switch.

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ST - 2

A HIGHLY SENSITIVE COLORIMETRIC AND FLUOROMETRIC SENSOR FOR THE DETECTION OF CYANIDE

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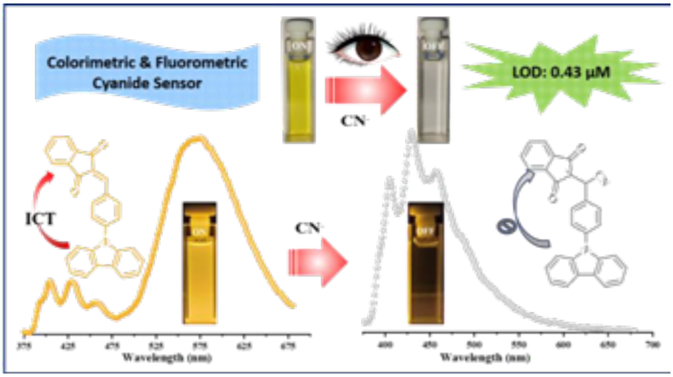

Cyanide ion (CN^-) is highly toxic and poisonous to humans, animals, and the environment. Even its low dose can be lethal to humans as well as aquatic life. Many plants, fruits and microorganisms contain mild to moderate quantities of cyanide ions, i.e., seeds of apples and apricots, cassava and sprouting potatoes, lima bean and almonds, etc. Cyanide ions can be entered in to the body through skin, lungs and gastrointestinal tract, etc., and causes headache, dizziness, high heart-beat, breathlessness, severe vomiting, and so on. According to the world health organization (WHO), the acceptable limit of cyanide ion (CN^-) concentration in portable water must be less than 1.9 µM or 0.2mg/L. Even though CN^- ion is highly lethal to the human body and aquatic life, it has been exploited in wide variety of applications such as insecticides, pesticides, metallurgy, electroplating, polishing industry (silver and gold), chemical and plastic industry (vinyl and polyurethane), leather tanning, petrochemical, etc. Hence, cyanide ion detection requires immediate attention for developing a rapid and efficient sensor that could be utilized to avert fatalities and also safe guarding the environment. Presentation will cover a few basic mechanisms of cyanide detection probes and recent research findings of my research group. Synthesis, photophysical properties of an ICT molecule and its application in detecting cyanide in Tapioca(cassava) would be discussed during my presentation.

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ST - 3

VISION OF FUNDAMENTAL PROTON AND ELECTRON TRANSFER: ADVANCING FROM SPECTROSCOPY TO BIOELECTRONICS

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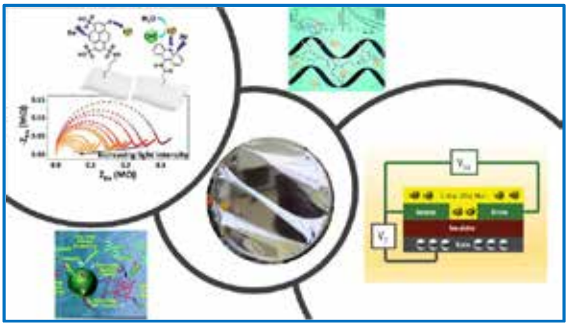

Figure 1: Modification and application of free-standingprotein-basedbiopolymer

Protons and electrons are the elementary currencies of nature, and their transport is an essential driving force of many key biological processes. Nature utilizes proteins to transport protons across the membranes, for example, proton channels in bioenergetic systems such as ATP synthesis. In solid-state conducting devices,protonic and electronic conductance play an important role for the development of bioelectronic devices. Recently, we have explored the from short range to long-range electron and proton transfer mechanism across the free-standing protein-based biopolymer with myriad uses of ultrafast spectroscopy and solid-state AC and DC bias driven electrical measurements where proteins are the main proton and electron mediators in this circuits. Moreover, advanced spectroscopy is employed for exploring the microenvironment of proton and electron transfer channel and deciphering the mechanism of proton and electron conduction mechanism across the biopolymer. This vision of protein-mediated long-range charge diffusion brings us far from biology to the bioelectronic fields and introduction to our main research to develop bio-optoelectronic devices. In this regard, we explored the fundamental mechanism of electron and proton transfer and bias-driven conductivity via the following modifications (a) chemical modifications of functional group (b) surface modifications with light modulated probe (c) doping of photosensitizer toward the formation of mixed conducting biomaterials (Figure 1) [1-3]. Thus, a detailed understanding of the complete picture of the carrier transfer mechanism across the biopolymer is only possible by combining uses of advanced optical study and electrical study. Here the innovation of a novel configuration of bioelectronics with high spectral and temporal resolution is a unique approach towards the resolving of perennial problem carrier transfer mechanism across the biopolymer that will bring it one step further towards the "**spectroscopy to bioelectronics**".

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ST - 4

RADIOIMMUNOTHERAPEUTIC AGENTS FOR TARGETING HER2 OVEREXPRESSING CANCERS

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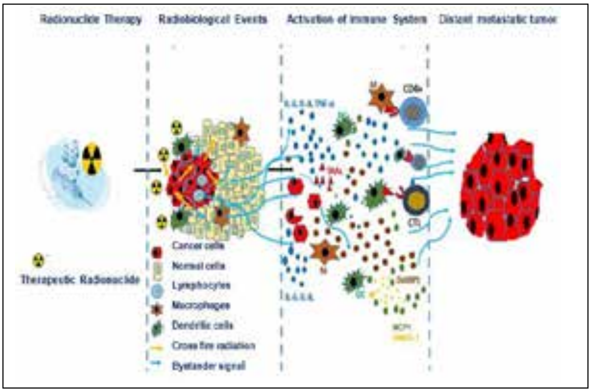

Figure 1. Schematic representation of Radiation linduced Biologic Bystander Effects (RIBBEs) observed with Radioimmunotherapeutic agents

Advanced solid tumors, including breast, ovarian, and gastric cancers, frequently overexpress the human epidermal growth factor receptor 2 (HER2), leading to aggressive disease progression and poor prognoses. To address this challenge, radioimmunotherapy (RIT) with radiolabeled antibodies was investigated to elucidate its therapeutic mechanisms and radiobiological phenomena, such as radiation-induced bystander effects. To develop a radioimmunotherapeutic agent targeting HER2-positive cancers, the FDA-approved antibody Trastuzumab was conjugated with the chelator CHX-A″-DTPA for radiolabeling with ^{90}Y (β-emitter) and ^{177}Lu (β-/γ-emitter). Additionally, ^{125}I (Auger electron emitter) was directly attached to Trastuzumab using an electrophilic substitution reaction. The radiobiological properties of these targeted radionuclide therapeutic agents were evaluated through media transfer experiments.

The radiolabeled antibodies exhibited high affinity, specificity, and immunoreactivity towards HER2 receptors. In HER2-overexpressing tumor-bearing mice, the radioformulations demonstrated significant uptake and retention in tumors. Under *in-vitro* conditions using HER2-overexpressing cell lines, all three radioimmunoformulations induced notable bystander toxicity. Furthermore, estimation of total cellular reactive oxygen species (ROS) suggested that ROS might play a critical role in mediating bystander effects in unirradiated cells. Understanding the mechanisms of action and radiobiological phenomena associated with radioimmunotherapeutic agents offers valuable insights. This knowledge could enhance the efficacy of treatments for solid tumors, providing a promising strategy to reduce side effects and overcome resistance to conventional therapies.

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ST - 5

RESOLVING THE ROLE OF SOLVENT POLARITY, VISCOSITY AND HYDROGEN-BONDING IN THERMALLY ACTIVATED DELAYED FLUORESCENCE

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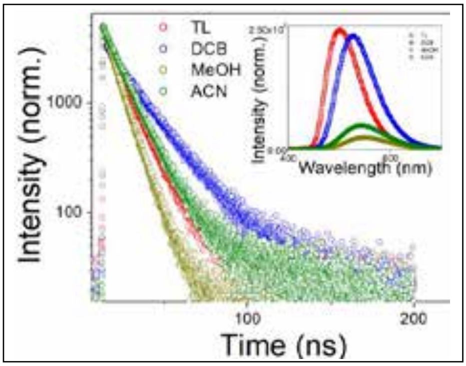

Figure 1: Effect of solvent on fluorescence lifetime. Inset shows it'seffect onfluorescence intensity.

Design and development of light emitting devices has received widespread attention in optoelectronic technologies. In a typical electroluminescent device, electrical excitation creates emissive singlet and nonemissive triplets in 1:3 ratio. However, for maximum quantum efficiency, both singlets and triplets need to be harvested. Thermally activated delayed fluorescence (TADF) has revolutionised display technology owing to minimal energy gap between the singlet and triplet excited states. This enables reverse intersystem crossing (rISC), a process where non-emissive triplet excitons are thermally up-converted into emissive singlet states. Efficient TADF emission requires solvent environment with both optimal polarity that could minimise the singlet-triplet energy gap and optimal viscosity that could facilitate the required intramolecular vibrations for efficient rISC [1,2]. Recent studies also highlighted the importance of intramolecular hydrogen-bonding in TADF molecules for providing high molecular rigidity and significantly impacting the singlet-triplet energy gap and rISC[3].However the role of solvent environment on TADF emission reported so far are typically combined effect of all these parameters thereby making it difficult to resolve their individual contributions. Here we have performed a systematic and detailed investigation of TADF emission in a range of solvents with different polarity, viscosity and hydrogen-bonding environment sutilising both steady-state and time-resolved optical spectroscopic tools. Comparing emission intensities and their lifetimes (see data in Figure 1 for only four solvents), we have been able to resolve the role of individual environmental factors in TADF emission. Novel insight thus generated will be useful for optimising the right environment that will significantly boost TADF emission in optoelectronic devices.

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Thesis Presentation (TH)

TH - 1

HYDROGEN BONDING REGULATED SELF-ASSEMBLY OF (MACRO) MOLECULES AND FUNCTIONAL MATERIALS

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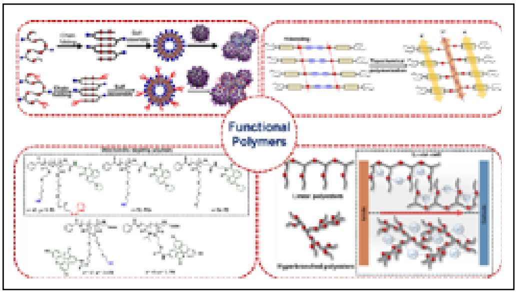

Figure 1. Schematic showing different aspects of functional polymers explored in the thesis.

In this thesis, we have described different types of functional polymers, including amphiphilic polyurethanes,polydiacetylenes, polyesters and polymethacrylates and depending on their self-assembly and intrinsic properties, have been applied to different fields. In the first part, functional amphiphilic polyurethanes have been explored in terms of their self-assembly through intra-chain H-bonding and chain folding and applied as antiviral polymers due to their excellent surface anionic sulfate group display, which helps them to interact with the viral receptors, blocking them to penetrate the host cell anymore[1]. In connection with the antiviral polymers, polymethacrylates with pendant as well as chain end functionality have been synthesized and tested for their cellular uptake behaviour, revealing different internalization patterns for differently functionalized polymers.Then the discussion slightly shifts from polymers for biological applications to polymers for potential utilization in the field of optoelectronic and energy devices, diacetylene monomers with appended naphthalene di-imide (NDI) unit has been synthesized which, in non-polar solvent tetrachloroethylene, self-assembles through H-bonding among the amide groups and π-stacking between the NDI chromophores, followed by topochemical polymerization by UV irradiation, which not only stabilized the supramolecular assembly but also generated a donor-acceptor heterojunction with hole transporting polydiacetylene backbone and electron transporting π-stacked NDI chromophores, making the system a unique organic semiconductor having both p-type and n-type properties which can be utilized for future optoelectronic applications[2]. In the last work described in the thesis, linear and hyperbranched polyesters have been synthesized through 100% atom efficient thiol-acrylate Michael addition reaction and tested for potential application as solid polymer electrolytes due to their Li-ion conducting properties[3].

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TH - 2

DEVELOPMENT OF POLYMER BASED COMPOSITES FOR EXTRACTION OF RADIONUCLIDES

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The rapid industrialization and escalating human activities have profoundly impacted our environment, generating waste streams laden with hazardous substances such as toxic dyes, heavy metals, and radionuclides. Among these, nuclear waste containing radioactive contaminants poses significant environmental and health risks. This research focuses on leveraging polymer-based materials for waste management, emphasizing the synthesis and application of novel polymer composites to efficiently extract radionuclides from diverse waste streams [1].

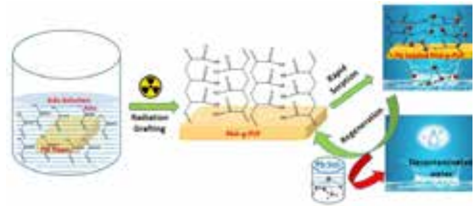

Figure 1. Radiation Induced Mutual Grafting of PAA over Puf.

A bifunctional chelating sorbent was developed by incorporating amine and amidoxime functional groups into cross-linked polyacrylonitrile (PAN) beads [2]. These beads achieved a saturation sorption capacity of approximately 45 mg/g for uranyl ions and performed effectively across a wide pH range (1–10). The study also introduced Zeolitic Imidazolate Framework-67 (ZIF-67) integrated into polyether sulfone (PES) beads through a phase inversion technique, yielding ZIF-67@PES composites. This composite improved stability, reusability, and operational simplicity, making the materials well-suited for column-mode uranium extraction from simulated seawater. For radioactive Cs^+ removal, a sand-based adsorbent was synthesized by coating natural sand with CoHCF using a deep-coating technique. Batch adsorption studies demonstrated a Cs^+ ion sorption capacity of approximately 5 mg/g across a pH range of 1–10, presenting a cost-effective solution for environmental safety. Lastly, the research introduced acrylic acid-grafted functionalized polyurethane foam (PAA-g-PUf) for the removal of lead ions from aqueous waste streams. This sorbent achieved a remarkable sorption capacity of 257 mg/g, reaching saturation within 10 minutes, and exhibited excellent reusability over five cycles.

The findings presented in this thesis highlight innovative polymer-based strategies for tackling the challenges of nuclear waste management. These materials demonstrate exceptional sorption performance, operational efficiency, and reusability, contributing significantly to environmental remediation and advancing sustainability efforts.

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TH - 03

TUNING FLUORESCENCE BLINKING AND DARK FRACTIONIN QUANTUM DOTS FOR SINGLE PHOTON SOURCE

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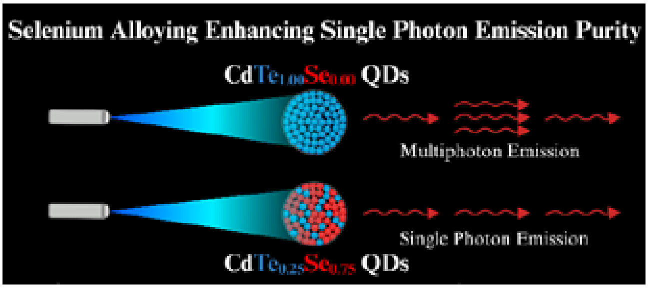

Single photon sources (SPS) are obvious requirement for the quantum technologies which have been revolutionized in recent years due to their superior applications in quantum technology, such as quantum computing, quantum communications, quantum sensing, metrology and quantum information processing. Unfortunately, most of the available SPS lose quantum coherence due to thermal fluctuations, electromagnetic fields, and other interacting environmental factors. As a result, the majority of the SPS are often operated at ultra-low temperatures (milliKelvin to a few Kelvin) to suppress environmental factors. Therefore, the development of room temperature SPS has now boosted up for the next generation quantum technology by circumventing the above issues. Quantum dots (QDs) have recently been reported as promising materials, such as SPS, at room temperature. Here, by optimizing the single particle optical properties of a series of $CdTe_xSe_{1-x}$, we provide an efficient SPS with increased single photon purity. The data revealed that second order photon correlation, $g^2(0)$ value decreases substantially with increasing the amount of selenium (Se) in CdTe QDs. This was accompanied by an increased photon count rate, substantially reduced fluorescence intermittency, and extended single particle ON-time. The increased single photon emission is attributed to very fast electron trapping to dense trap states, which suppresses the multiexciton recombination.

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Oral Presentations (OP)

OP - 1

INVESTIGATION OF B^{q+} ION INDUCED L- SHELL X-RAY RELATIVE INTENSITIES OF $_{70}$Yb

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In this paper, we present the relative intensity ratios, $I_k/I_{L\alpha}$ (k = L_{ℓ}, L_{α}, $L_{\beta13,6}$, $L_{\beta2,15'7,9,10}$ $L_{\gamma1,5}$, $L_{\gamma2,3'8}$, $L_{\gamma4}$), for $_{70}$Yb induced by the bombardment of 30 and 45 MeV B^{+q} ions. The measurements were performed using the atomic physics beam line of the 16UD Pelletron Accelerator at the Inter-University Accelerator Centre (IUAC), New Delhi. Thin targets evaporated on an ultrapure carbon backing having thickness ~20μg/cm^2 were bombarded by incident ion beam. The targets, mounted on a steel ladder, were positioned in an evacuated (< 10^{-6} Torr) scattering chamber at 45° angles to both the beam direction and the SDD X-ray detector. The L X-ray spectra were separately deconvoluted into various components of the L X-ray lines using a computer code ORIGIN, after subtracting the background spectra recorded using blank carbon backing as target. The experimental results were compared those calculated using boron ion induced L_j (1-3) sub-shell ionization cross sections based on the the ECPSSR [1] model, the X-ray emission rates based on the Dirac-Hartree Slater (DHS) model [2], the fluorescence and Coster-Kronig yields based on Dirac-Hartree Slater (DHS) model [3]. The differences observed between the present measured and calculated experimental values could be due to multiple-ionization induced in the investigated elements by the incident boron ions. These findings contribute to a deeper understanding of atomic interactions in ion-beam-induced X-ray emission processes and provide valuable data for applications in materials science and nuclear physics.

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OP - 2

IMPACT OF ELECTROLYTEATTHE UNCHARGED POLYMER/WATER INTERFACE: OBSERVEDBY SUM FREQUENCY GENERATIONAND RAMAN SPECTROSCOPY

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Polyethylene glycol (PEG) is a versatile water-soluble non-ionic polymer having applications in Li-ion batteries, water-splitting, protein precipitation, anti-biofouling, and drug delivery. These applications crucially depend on the interaction of PEG with water at its surface, which is found to be a function of its molar mass and the ionic strength of the solution. However, the molecular mechanism underlying this dependence on molar mass and ionic strength remains unknown.

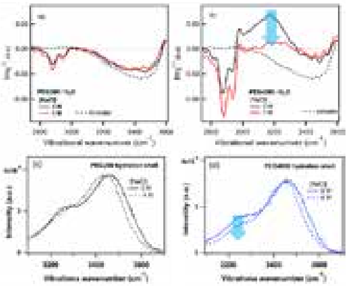

Figure 1. Imc(2) spectra (a & b) and Raman-DS-SCF extracted hydration shell spectra (c& d) for PEG200 and PEG4000

In this study, we explored the structural and orientational changes of water at the PEG/water interface using PEGs with varying molar masses and ionic strengths. This was done through heterodyne-detected vibrational sum frequency generation spectroscopy (HD-VSFG) and Raman difference spectroscopy with simultaneous curve fitting analysis (DS-SCF)[1]. HD-VSFG selectively probes interfacial molecular vibrations and orientation, while Raman-DS-SCF provides hydration-related vibrational spectra of water. The combined results offer molecular insights into water's behavior and structural changes at the PEG/water interface.The OH stretch imaginary-$c^{(2)}$ spectra (Im$c^{(2)}$; $c^{(2)}$is the second-order electric susceptibility of the interface) of the low molar mass PEG (PEG200)/water interface shows a negative band in 3000 -3600 cm^{-1}, similar to that of the air/water interface (Figure 1a). This reveals that the average hydrogen-bond (H-bond) structure and net hydrogen-down interfacial water (H-down i.e., the interface water-Hs' are oriented towards the aqueous bulk) of the pristine air/water interface, do not change appreciably in presence of PEG200. However, for the high molar mass PEG4000, the Im $c^{(2)}$spectrum adopts a positive sign around 3200 cm^{-1} and a negative sign around 3450 cm^{-1}, revealing the simultaneous presence of H-up and H-down oriented water (Figure 1b). On increasing the ionic strength (1.0 M NaCl), the structure and orientation of water at the PEG4000/water change, but not so at the PEG200/water (red curves Fig 1a and 1b). Specifically, the response of the strongly H-bonded and H-up oriented water (positive band around 3200 cm^{-1}) decrease while the relatively weakly H-bonded and H-down oriented water (negative band around 3450 cm^{-1}) remain unchanged (Fig 1b). Raman-DS-SCF extracted OH stretch spectra of water in the hydration shell of PEG200 and PEG4000 (Fig 1c and 1d) are also positively correlated with the corresponding HD-VSFG results. Thus, the combined results suggest that the structure and oriented water at the PEG/water interface is dependent on the molar mass of PEG and are governed by the interfacial hydration of PEG, instead of long range orientational order via the formation of an electric double layer. In presence of NaCl, the hydration shell of the ether-oxygen of surface adsorbed PEG4000 is selectively disrupted, leading to the loss of 3200 cm^{-1} band and the corresponding H-up oriented water (red curve Fig 1b). This observation implies that the water trapping ability of high molar mass PEG decrease in presence of electrolyte, which may reduce protein precipitation ability of the PEG.

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OP - 3

FROM MOLECULAR DESIGN TO CELLULAR TARGETING: THE MULTI FUNCTIONALITY OF BROMO BENZOTHIADIAZOLE-BASED FLUOROPHORES

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This work investigates the synthetic, photophysical properties, theoretical aspects, Aggregation-Induced Emission (AIE) behaviour, and bioimaging potential of π-conjugated 4-bromo phenylethynyl-2,1,3-benzothiadiazole derivatives (BrBTDs) with various electron-donating (ED) substituents at the para position of the phenylethynyl moiety. Due to the electron-deficient nature of 2,1,3-benzothiadiazole, the presence of ED groups at the opposite terminal forms D-π-A fluorophores with unique photophysical properties and broad applications [1,2]. BrBTDs with strong ED groups (e.g., methoxy, *N*,*N*-diphenylamine, *N*,*N*-dimethylamine) exhibit significant Intramolecular Charge Transfer (ICT) behaviour in polar solvents, alongside local emission (LE) in apolar solvents, where LE shows a higher quantum yield than ICT emission. Theoretical TD-DFT calculations support the ICT behaviour observed in these compounds. These novel D-π-A fluorophores, display AIE behavior in THF/H_2O mixtures and exhibit bright solid-state emission. BrBTDTPA was further utilized to probe temperature-induced phase transitions in DMPC and DPPC lipid bilayers through fluorescence emission intensity and lifetime measurements. Additionally, BrBTDOMe served as a bioimaging probe to study the localization of cellular targets, specifically the endoplasmic reticulum (ER), in living cells.

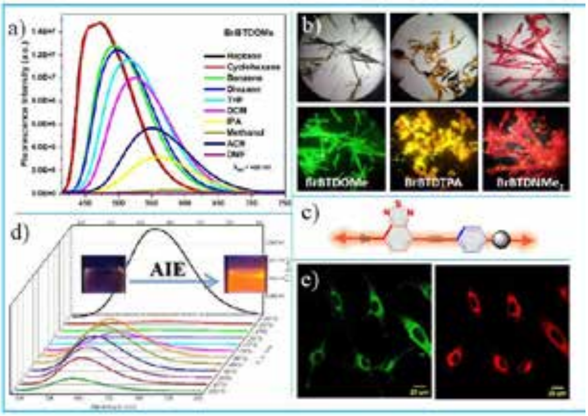

Figure 1. represents(a) solvatochromism of BrBTDOMe, (b) solid-state emission under microscope (upper panel: under white light, lower panel: under UV light), (c)a model structure of BrBTDs, (d) AIE feature of BrBTDTPA, (e) BrBTDOMe as a bioimaging probe specifically staining ER.

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OP - 4

EXCIMER FORMATIONDYNAMICS OF PYRENE IN A SUPRAMOLECULAR MATRIX

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Conventional silicon-based semiconductors have several drawbacks, including high manufacturing costs, low power efficiency, and high-temperature requirement for processing. On the other hand, metal-free π-conjugated organic semiconductors are more desirable for photonics, bioelectronics, and optoelectronics due to their flexibility, simpler processing, and biocompatibility.[1] However, these materials are often required in solid or aggregated states for device fabrications such as thin films. But in these states, conventional polycyclic π-conjugated chromophores like anthracene, perylene, and pyrene tend to experience strong π–π stacking interactions, energy transfer, and charge transfer processes, which reduce photoluminescence efficiency and hinder their practical use. [2]

We attempted to reduce the aggregation of pyrene in solid state by co-assembling it with a low molecular weight gelator. The gelator was synthesized by a one-step reaction from the cholesteryl chloroformate and pentaerythritol which yielded the co-gel. The co-gel was rapidly frozen using liquid nitrogen and then vacuum-dried to obtain a xerogel. [3] We investigated the photo-dynamics of pyrene in various states (concentrated solution, powder, and xerogel) using steady-state and time-resolved spectroscopy. In xerogel, pyrene showed enhanced fluorescence intensity compared to the solution and powder and exhibited excimer band in the range of 415 to 590 nm along with monomer emission. In case of concentrated solution, we observed one isoemissive point at ~443 nm which corresponds to direct interconversion of monomer to excimer. Whereas in case of powder pyrene, two iso-emissive points show that monomer is interconverting to excimer at ~445 nm and then relaxing to intermediate state (~485). However, pyrene in xerogel shows three iso-emissive points. These isoemissive points can be explained as monomer relaxing to intermediate state at ~418 nm then gradually decaying to form excimer at ~442 nm and subsequent appearance of third isoemissive point at ~423 nm probably due to longer lifetime of monomer as compared to excimer. These observations indicate involvement of multiple intermediates in the monomer-excimer transition in solid matrix.

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OP - 5

PYRENE BASED AIE-ACTIVE PROBE FOR SELECTIVE DETECTION OF PICRIC ACID THROUGH THE INNER FILTER EFFECT CHANNEL IN AQUEOUS MEDIUM

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The development of pyrene derivatives possessing the AIE feature have emerged as an intriguing area of research with potential applications in several domains. In the present study, we designed and developed an AIE active pyrene derivative for picric acid sensing in an aqueous medium. In comparison to pristine pyrene, the synthesized pyrene derivative has a lower bandgap energy as a result of the intramolecular charge transfer between pyrene and 4-(methylthio)-2-oxo-2*H*-pyran-3-carbonitrile. The synthesized probe demonstrates a moderate level of fluorescence when dissolved in a solution, and it has exhibited a remarkable emission caused by aggregation at higher water percentages. The aggregates have shown enhanced fluorescence quantum yield and lifetime, rendering them a more suitable option for sensor applications and so they were effectively employed as a fluorescent probe for the detection of picric acid in an aqueous medium. The probe exhibited a notable level of selectivity and sensitivity towards picric acid, as evidenced by its low detection limit of 4.47 nM. Moreover, the quenching mechanism was ascribed to the inner filter effect, providing supporting evidence from both experimental and mathematical calculations. The findings indicate that the probe has potential as a feasible choice for a picric acid sensor.

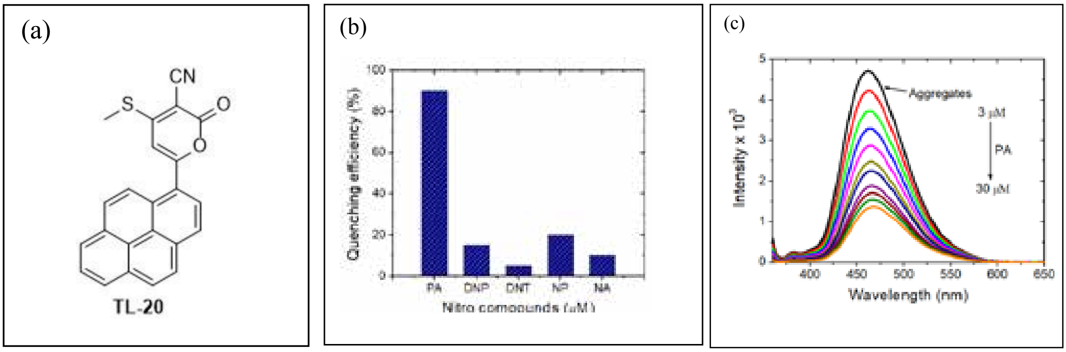

Figure 1. (a) Structure of TL-20 (b) (a) Selectivity plot of TL-20 to various explosive (c) Emission response to PA.

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OP - 6

SMALL FLUORESCENT PROBESFOR PESTICIDES DETECTIONIN REAL-LIFE SAMPLES: A PREVENTIONOF PESTICIDE POISNINGATTHE DOORSTEP

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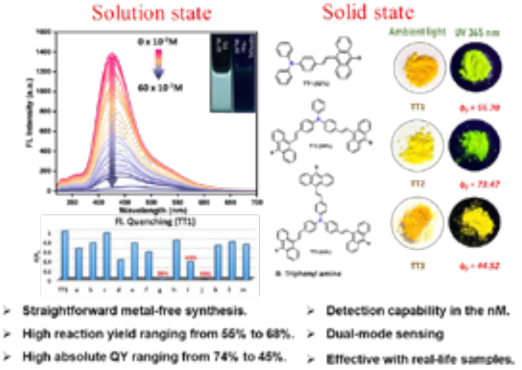

- Straightforward metal-free synthesis.
- High reaction yield ranging from 55% to 68%.
- High absolute QY ranging from 74% to 45%.
- Detection capability in the nM.
- Dual-mode sensing
- Effective with real-life samples.

Figure 1.Thoughtful design, synthesis, and implementation of TT1, TT2, and TT3. As a dual mode pesticide detector.

Over the past few years, a significant upsurge in agricultural productivity has been attributed to the refinement of water management techniques, progress in cultivation science, and the practical application of potent pesticides. The widespread use of diverse pesticides, including both organophosphates (OPs) and non-organophosphates (non-OP) remains a significant concern in India. In particular, pesticide use is prevalent among farmers and agriculture workers in rural agricultural areas. Many of them are poisoned by pesticides every year. Accurate monitoring of toxic pesticides is essential to protect the environment and food supplies due to their extreme toxicity.[1-3] In this context, triphenylamine-based three C_1, C_2, and C_3symmetrical molecules **TT1, TT2**, and **TT3** were easily synthesized *via* base-mediated Horner-Wadsworth-Emmons reactions between corresponding aldehydes and phosphonates. Further, the photophysical properties of the dyes were investigated in solid and solution states. The **TT1** absorbs at λ_{abs}= 445 nm and emits at $\boldsymbol{\lambda}_{em}$= 531 nm with absolute quantum yield($\boldsymbol{\phi}_f$) of 44.52%, while **TT2** exhibited λ_{abs}= 440 nm and λ_{em}= 541 nm, and $\boldsymbol{\phi}_f$ of 74.47% . The **TT3** revealed λ_{abs}= 450 nm, λ_{em}= 538 nm, and $\boldsymbol{\phi}_f$ of 55.70%. These probes detect a few pesticides selectively in dual-phase efficiently (solid/solution) in the nM range. Additionally, mechanistic insights were investigated in detail. They were employed for onsite pesticide detection in real-life samples soil, leaves, and fruits. It offers a handy solution for the onsite detection of pesticides in the form of varnished buds or spray formulations. and show great potential as candidates for sensors accessible and useful for everyday applications.

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OP - 7

GAMMA-IRRADIATED PCL/CNT CHEMIRESISTORS FOR POLAR VAPOUR SENSORS

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Research has consistently demonstrated that in nanocomposites, the interface between the nanofillers and the matrix material significantly influences overall properties [1]. This is particularly evident in chemiresistive sensors, where the interaction at the nanofiller-matrix interface can profoundly affect the sensor's response to specific gases. This study investigated the effects of gamma irradiation on polycaprolactone (PCL)/carbon nanotube (CNT) nanocomposites for acetic acid vapor sensing. Gamma irradiation introduces cross-linked networks within the nanocomposite, thereby modifying the electron conduction pathways and enhancing the sensor's performance [2]. PCL and CNTs were combined using a chloroform-based solvent processing method, with 2% by weight of CNTs incorporated into the PCL matrix. The fabricated sensors were evaluated using IDEs in a sealed 2L chamber. Resistance changes were monitored in real-time to assess the sensor response. The results revealed that optimal gamma irradiation at 25 kGy led to a significant enhancement in the chemiresistive response of the PCL/CNT nanocomposite towards acetic acid vapor (Fig.1). The sensor exhibited exceptional stability over extended periods (30 minutes), excellent reproducibility across multiple cycles, and consistent performance even after month. Notably, the irradiated nanocomposite demonstrated a superior sensitivity to acetic acid vapor, at 2.26 ppm. These findings align with our previous research on the impact of gamma irradiation on nanocomposite-based sensors [3].

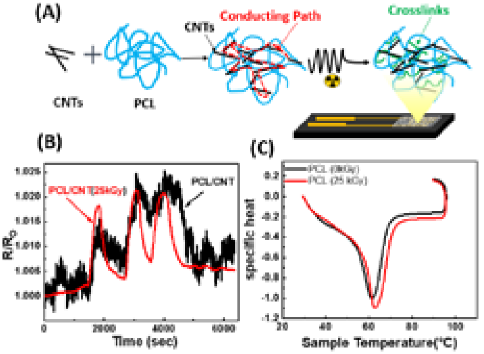

Figure 1. (A) Synthesis scheme of Irr-PCL/CNT composite (B)Sensing response of PCL/CNT & Irr-PCL/CNT to 2.26 ppm AcOH vapours (C)Impact of the Gamma irradiation on the melting behaviour of the PCL

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OP - 8

HIGHLY ACCELERATED PHOTOCYCLOADDITION OF CYANOSTILBENE DIMERS IN AQUEOUS MEDIA

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Supramolecular photochemistry has emerged as an exciting field in recent decades providing unique control on the regio- and stereo-selectivity in photochemical transformations which are difficult to accomplish through conventional solution state photochemistry. We have recently studied the photochemistry of dicationic cyanostilbene (CS) derivatives in which a single CS unit was flanked by two alkyl chains of variable lengths at the termini. Interestingly, we observed that these derivatives underwent photoisomerization (trans-cis) and photocyclization in solution and in the self-assembled state in aqueous media. However, photocyclization was more efficient in the self-assemblies [1]. Herein, we report new dimeric CS derivatives in which two CS chromophores are connected via variable aliphatic linkersas shown in Figure 1. It was found that the choice of solvent dictated the conformation of these CS dimers. In DMSO and methanol, they were present in molecularly dissolved state with monomer-like emission and resulted in slow trans-cis isomerization reactions under 365 nm light irradiation. On the other hand, in aqueous media, they were present in a folded state generating intramolecular excimer emission. The intramolecularly folded state led a highly accelerated 2+2 photocycloaddtion. The flexible linker between the two chromophores was varied from butylene (C4) to hexadecylene (C16). Interestingly, even with the longer linkers, intramolecular excimer formation and the [2+2] cycloaddition product were observed in aqueous media. The resulting nanomaterial was subsequently attached to a polymeric backbone for potential applications [2].

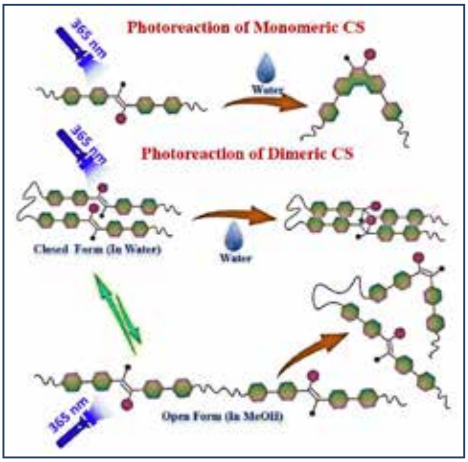

Figure 1 Top: Photoreaction of monomeric CS. Bottom: Molecular configurations and photoreactions of dimeric CS in different solvents.

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OP - 9

THE PHOTOCHEMICAL BEHAVIOUR OF OXYGEN MEDIATED SYNTHESIZED RADICAL

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Persistent radical are often hard to synthesize let alone in the presence of oxygen, but their unique electronic and magnetic properties make themselves worthy candidate in material science [1]. However, the rise of photo-induced synthetic transformations has emerged as a viable strategy to redefining classical organic synthesis in a sustainable manner [2,3]. In this work, we have synthesized the chromeno based radicals (JM_1) using oxygen as the oxidant under ambient conditions. This stable but kinetically controlled radical, JM_1 is characterized using single crystal-XRD and solid state X-band EPR and as well with spin trapping agents 5,5-dimethyl-pyrroline-N-oxide (DMPO). Further in solution state, this radical when exposed to either sunlight or LED light (405 nm), it initially showed change in color as it changes from colorless to yellow and then it again goes back to colorless within 60 min. This photo-induced transition in color is due to the formation of an intermediate in approach of forming thermodynamically stable radical (JM_2) from kinetically formed radical, (JM_1).

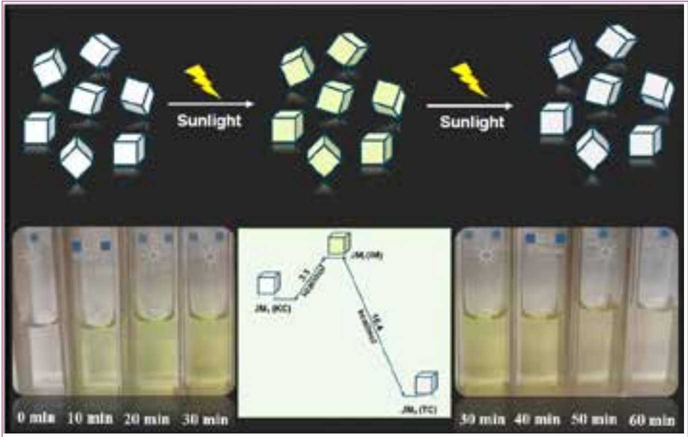

Figure 1. Pictorial description of conversion of kinetically controlled radical (JM1) to thermodynamically controlled radical (JM2) through an intermediate (JMi) using sunlight and the energy involved during the process.

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OP - 10

MOLECULAR LEVEL INSIGHTS ON AGEING MIXED UREA-MALONIC ACID AEROSOLS

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Atmospheric aerosols consist of various classes of organic compounds, which can originate from both natural and anthropogenic sources, such as ammonia, amines, and amides, or form in situ through atmospheric ageing processes, including the formation of dicarboxylic acids [1-2]. In this study, the inter-molecular interactions and humidity mediated evolution of chemical identities in mixed 1:1 urea-malonic acid (MA) aerosol have been investigated using in-situ micro-Raman spectroscopy.

During dehumidification, the pure urea and MA aerosols showed efflorescence RH (ERH) at 20% and 46%, respectively, while the mixed system effloresced at 49%RH, exhibiting urea like behaviour. Upon gradual drying of the mixed particles, the symmetric C=O stretch of COOH blue shifts to a distinct sharp band at 1740 cm^{-1} along with the appearance of symmetric stretch of carboxylate at 1380 cm^{-1}. Further, the appearance of two new bands at 1136 and 1500 cm^{-1} corresponding to –C-(NH) bending and -C-N-C stretching associated with new -C-(NH)-C(=O) bond, suggest new intermolecular interaction in the mixed particles.DFT based computational studies on the 1:1 mixed urea-MA condensation process showed formation of 3-oxo-3-ureidopropanoic acid as shown in following schematic.

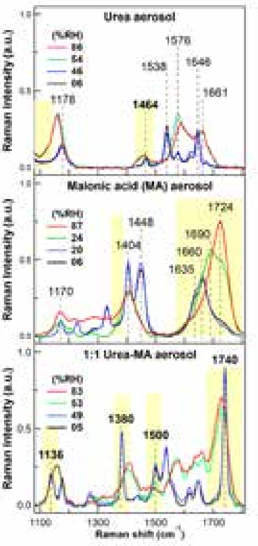
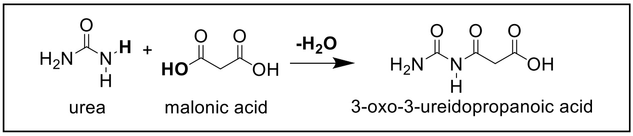


Figure 1. Aerosol Raman spectral changes during dehumidification.



Thus, observation of new chemical species in ageing urea aerosols has great relevance in the context of new particle formation.

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OP - 11

MAGNESIUM-PORPHYRIN, A CATALYST WITH ENORMOUS EFFICIENCYFOR THE PHOTOCHEMICAL CONVERSION OF GASEOUS CO_2INTOCYCLIC CARBONATESANDOXAZOLIDINONES

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Global warming is one of the most challenging problems for the mankind with an alarming rise in the sea level where Carbondioxide, the major green house gas, contributes predominantly to this world wide temperature rise. So, any chemical conversion by arresting CO2 in the form of a valuable chemical compound is of great importance and would be a significant stride towards a greener world. Carbon capture in terms of chemical reaction and sequestration is one of the most effective methods to abate atmospheric CO2 levels [1]. Various homogeneous and heterogeneous catalytic systems, including metal complexes, metal oxides, organocatalysts, ionic liquids, etc., have been already developed for the cycloaddition of CO2 with highly strained three-membered rings like epoxides, and aziridines [2]. Among these, metal complexes like metal salens, or metal porphyrins are much more superior due to their enormous catalytic efficiency. Employing a simple Mg-porphyrin metal complex as a visible light photocatalyst for the photochemical cycloaddition of CO2 with epoxides or aziridines to furnish various cyclic carbonates or oxazolidinones under solvent-free and at ambient conditions presents a promising strategy towards the abatement of global warming. This greener and sustainable approach applies to a wide range of substrates, including a library of terminal and internal epoxides and aziridines.

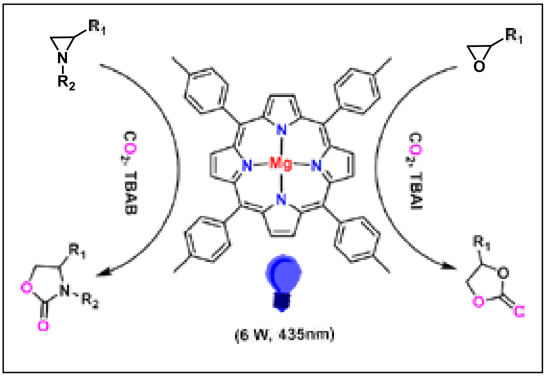

Figure 1. Schematic representation of Mg(II)-Porphyrin catalyzed photochemical cyclo-addition of CO_2 to furnish organic moiety.

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OP - 12

POSITION-DEPENDENT MODULATION OF INTERSYSTEM CROSSING IN IODO-FUNCTIOALIZED SALICYLIDENEIMINE-BORON COMPOUNDS

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Intersystem crossing (ISC) is the key factor to generate the molecular triplets, which can be significantly enhanced by the introduction of heavy atoms due to their ability to strengthen spin-orbit coupling (SOC) [1]. However, the influence of the heavy atom's position within a molecule on ISC efficiency remains largely unexplored [2]. In this study, we address this gap by investigating the ISC process in three positional isomers of an iodine-substituted Salicylideneimine-Boron compounds: 3ISB, 4ISB, and 5ISB. Using a combination of steady-state and time-resolved absorption and fluorescence spectroscopy, we observed that ISC efficiency varies notably between the isomers. The 3ISB isomer exhibited the most efficient ISC and triplet formation, followed by moderate efficiency in 5ISB and the least efficiency in 4ISB. Quantum chemical calculations suggest that SOC is not the only parameter governing the ISC process; C–X bond vibrations may also play a role in influencing ISC in such heavy-atom systems. These findings provide a deeper understanding of the positional dependency of ISC in heavy atom-modified molecules and offer valuable insights for the design of highly efficient triplet-state materials, which have broad applications in various fields such as organic electronics and photodynamic therapy.

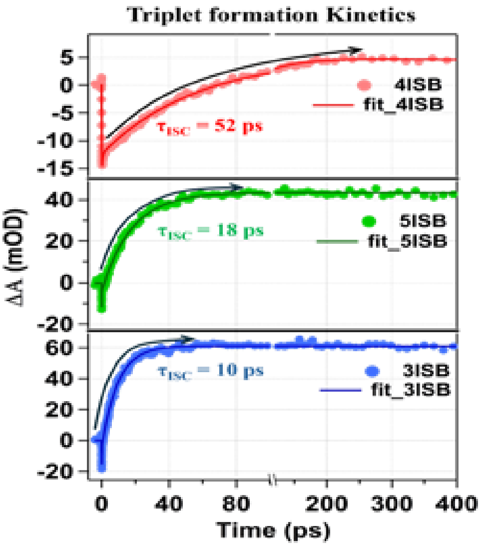

Figure 1.Triplet formation kinetics of positional isomers of iodo-Salicylideneimine-Boron compounds

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Radiation Chemistry Posters (RC)

RC - 1

QUALITATIVE AND QUANTITATIVE ANALYSIS OF FOOD PROCESSING TREATMENTS ON CLUSTER BEANS

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Table 1 Qualitative analysis of cluster beans

Phytochemicals	Control	Autoclaved	Irradiated	Cooked
Saponin	+++	+++	-	+
Quinone	+++	++	++	-
Phenol	+++	++	++	-
Steroid	+++	+++	++	+
Flavonoid	-	+	+++	++
Tannin	+++	+	-	-
Terpenoid	+	++	+++	+++

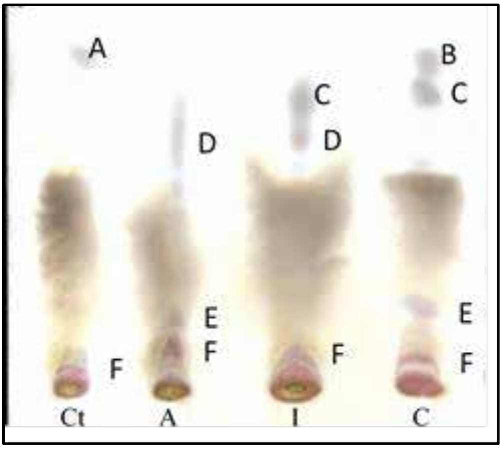

Figure 1. TLC of processed cluster beans

Cluster bean (*Cyamopsistetragonoloba*) is an annual Indian legume crop with numerous health benefits. Food processing increases the release of phytochemical but also lead to faster food spoilage [1]. In the present study cluster beans were processed by irradiation, cooking and autoclaving These processed samples (10% homogenate) were innoculated with food spoilage *Aspergillus* and *Mucor* species. The samples were incubated at ambient temperature No mold growth was observed initially. The spoilage organisms *Mucor* and *Aspergillus* spoilt the cooked, autoclaved and irradiated samples stored at ambient temperature in 3, 3 and 7 days respectively while control samples spoilt after 11days. Qualitative analysis of cluster beans showed presence of high presence of saponin, quinon, phenol, steroids, tannin moderate presence of terpenoid. A decrease in quinones and phenols was observed in autoclaved and irradiated samples while they were absent in cooked samples. The processed samples also showed increased presence of steroids and terpenoids. The most interesting observation was presence of flavonoids in the order irradiated > cooked > autoclaved which are absent in control samples. TLC analysis showed compound A present in control and cooked sample probably has been lost or broken on processing as it is not observed in autoclaved and irradiated samples. A new compound D is observed in autoclaved and irradiated samples. The irradiated sample also shows another

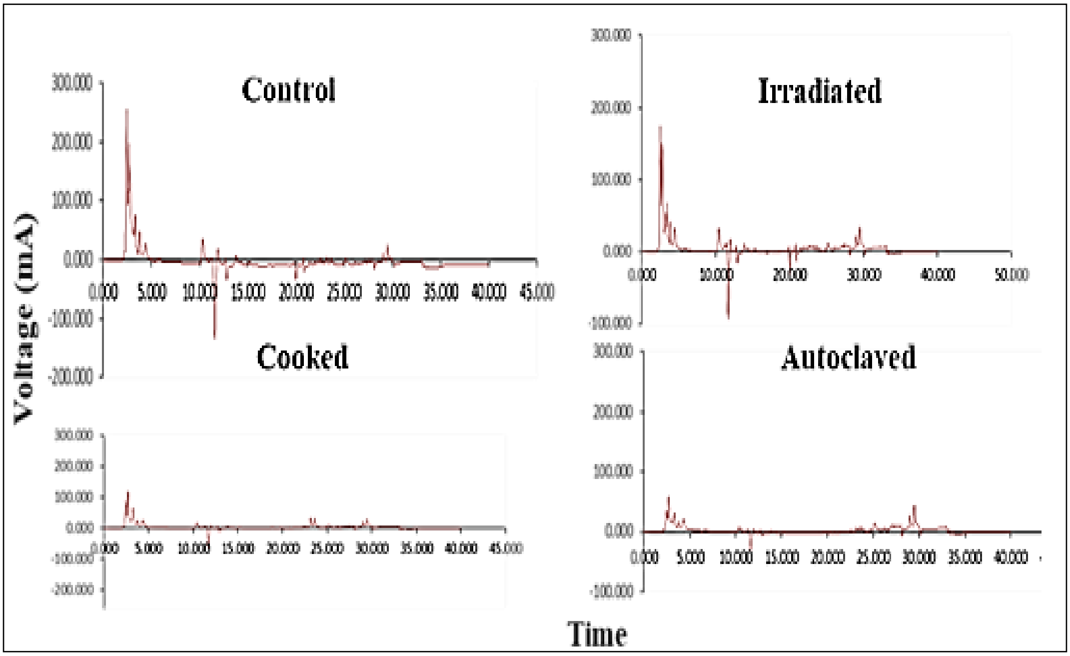

Figure 2 HPLC of processed cluster beans

distinct compounds B. Cooking has broken the phytochemicals in three more compounds (D, E and F). Increase in antioxidant activity in irradiated (94.04%) and autoclaved (85.49%) sample as compared to control (73.85%) was also noted. Further HPLC analysis showed presence of gallic acid, chlorgenic acid and kaempferol in control sample with decreased levels in irradiated samples and absence of these compounds in autoclaved and cooked samples. Thus, food processing by irradiation shows least damage to the phytochemicals as compared to heat treatments and is a better method for preservation of cluster beans at ambient temperature.

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RC - 2

FREE RADICAL INDUCED OXIDATION OF URACIL ORCHESTRATED BY GOLD NANOPARTICLES

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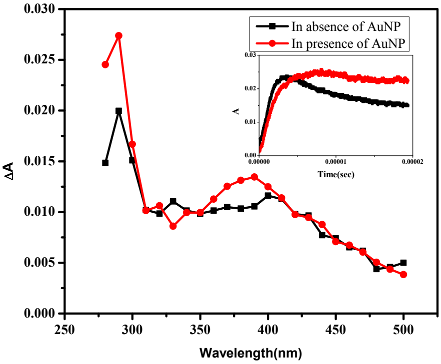

Figure 1. Transient absorption spectra at 3ms in presence (Red) and in absence of Au NP (Black) Inset: Formation trace monitored at 280 nm in presence and absence of Au NPs.

Magnified use of nanotechnology in various fields viz. medical, electronics, sensing and many more lead to intentional or unintentional exposure of nanoparticles (NPs) in biological systems. This demands the study of the interaction of NPs with biomolecules as they are the major targets for cellular oxidants that cause alterations in the pyrimidine base pairs. The catalytic role of Gold Nanoparticles (AuNPs) in the $^{\cdot}$OH-induced oxidation of Uracil (U) was investigated using steady-state and pulse radiolysis techniques. AuNPs were synthesised by Creighton's method and subsequently characterised by UV-Vis spectroscopy, DLS and TEM to determine morphology and size [1]. Pulse radiolysis studies were carried out to elucidate the interaction mechanism of AuNPs with U at different pH and compared with the $^{\cdot}$OH radical reaction with U [2]. The transient species produced showed two prominent absorption maxima centred at 280 and 320 nm respectively. The formation trace (Fig. 1, inset) recorded at 3μs suggests the stabilisation of the transient species formed in the presence of AuNPs. The first order rate constant calculated inferred the reaction to be diffusion-controlled and influenced by AuNPs.

Steady State Radiolysis deduced the protective influence of AuNPs as $-G_U$ was estimated to be 28% lower in the presence of AuNPs. The stable products formed viz. isobarbituric acid and 5-hydroxy Uracil were analysed by HPLC. The findings will be discussed in detail.

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RC - 3

ETHYLENE VINYL ACETATE (EVA) AND BARIUM SULPHATE ($BaSO_4$) COMPOSITES AS X-RAY SHIELDING

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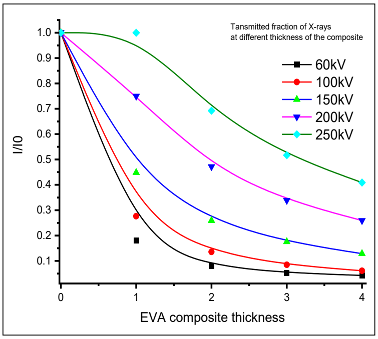

Figure 1. Transmitted fraction of X-ray with thickness

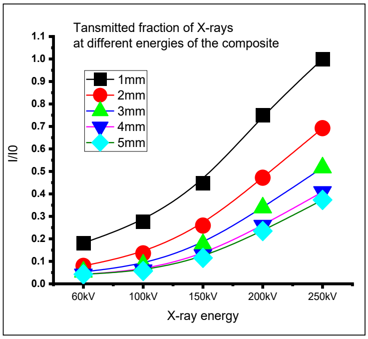

Figure 2. Transmitted fraction of X-ray with energy

Recent research has focused on developing composite-based protective materials that can be molded into various shapes without requiring high temperatures. These materials are useful for creating protective clothing to shield radiation workers and patients from radiation. In this study, Ethylene Vinyl Acetate (EVA) - Barium Sulphate ($BaSO_4$) composites were developed with 500 parts per hundred of rubber (phr) of Barium Sulphate. EVA served as the base matrix, while Barium Sulphate acted as the filler. The polymer composites were molded into sheets measuring 10 x 10 cm^2 and 1.0 mm in thickness. The density of the composites was measured to be 2.6 g/cm^3.

Attenuation studies of the composites were conducted using a Siemens Polydorus-LX high-frequency generator X-ray machine (maximum 450 kV, maximum 800 mA), with a kV variation of ± 1 kV. The percentage transmission of the developed samples at 60-250 kVp for different thicknesses and with 500 phr of Barium Sulphate loading is depicted in Graphs 1 and II.

The results demonstrate that with 500 parts per hundred of rubber (phr) loading of Barium Sulphate in Ethylene Vinyl Acetate (EVA), the composite material achieves over 80% attenuation in the energy range of 100 keV while retaining flexibility. This flexibility allows the material to be manufactured into various forms such as aprons, vests, thyroid collars, and gonad shields. Such radiation shield materials are particularly useful for objects with curved surfaces in low-energy gamma/X-ray fields, providing optimal radiation protection for both workers and patients.

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RC - 4

PREPARATION OF PVDF-GMA ANION EXCHANGE MEMBRANE BY GAMMA RADIATION GRAFTING

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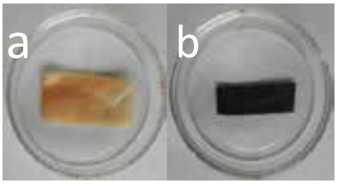
Hydrogen is the most prevalent element in the universe; however, its primary production method is through natural gas, categorizing it as gray and blue hydrogen. In contrast, green hydrogen is generated from renewable sources such as solar and wind energy. Unlike cation exchange membranes, anion exchange membrane (AEM) electrolysers utilize cost-effective electrode materials, including nickel and cobalt, which facilitate the production of high-purity hydrogen at elevated pressures. Nevertheless, the stability of AEMs poses a challenge due to the instability of quaternary ammonium groups, which can significantly reduce their lifespan, particularly at high temperatures. The objective of the present study is to create stable and durable AEMs via gamma radiation-induced grafting. Poly(vinylidene fluoride) (PVDF) demonstrates outstanding thermal and mechanical characteristics, rendering it an ideal candidate for the fabrication of efficient ion-exchange membranes. The material can undergo grafting through gamma radiation and chemical methods [1] using appropriate monomers to produce an ion-exchange membrane.



a) PVDF Membrane before quaternization
b) PVDF Membrane after quaternization

Figure. 1 membrane images

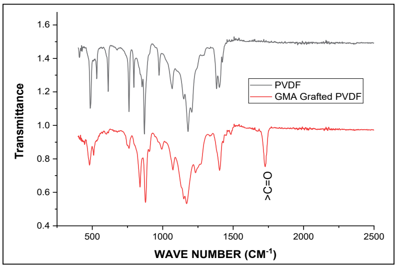


Figure. 2 IR Spectra of PVDF and GMA Grafted PVDF

In the current investigation, the grafting of glycidyl methacrylate (GMA) onto the PVDF macromolecule was achieved through gamma radiation in a solution, without the use of any cross-linker. This was followed by a quaternization process to produce PVDF-GMA anion exchange membranes. The ratios of PVDF to GMA and the total radiation dose were adjusted to optimize the grafting conditions. The membranes were characterized using a variety of techniques, including FTIR, TGA-DSC, SEM, and contact angle measurements. Grafting was confirmed by the presence of the >C=O ester group peak of GMA at 1725 cm^{-1}, as observed in ATR FTIR analysis. The resulting PVDF-GMA anion exchange membrane exhibited a conductivity of 2 mS cm^{-1} at room temperature and 12 mS cm^{-1} at 60°C for a PVDF:GMA ratio of 4:3. The membrane demonstrated excellent conductivity and thermal stability.

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RC - 5

DEVELOPMENT OF AMIDOXIME-MODIFIED BIOPOLYMER COMPOSITES FROM RADIATION-SYNTHESIZED PAN FOR URANIUM EXTRACTION

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Uranium plays a crucial role in nuclear power generation and isotope production, but its natural sources are limited, being found in trace amounts in rocks, soil, and seawater. Despite its importance, uranium is radioactive and toxic, posing chemical, biological, and radiological risks to living organisms [1]. Effective treatment of uranium-contaminated effluents is essential. Various methods, such as solvent extraction, chemical precipitation, membrane filtration, and electrochemical techniques, have been developed for uranium removal. However, solvent extraction, though widely used, has limitations like high cost, third phase formation, and secondary waste generation, making it less suitable for large waste volumes with trace uranium concentrations. Solid-phase extraction offers a more practical, eco-friendly, and cost-effective alternative for handling large volumes of waste [2].

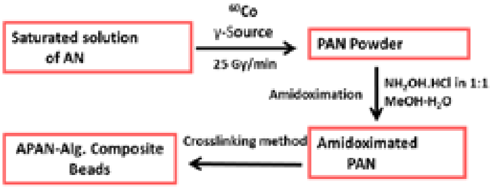

Figure 1. Radiation induced synthesis of PAN powder

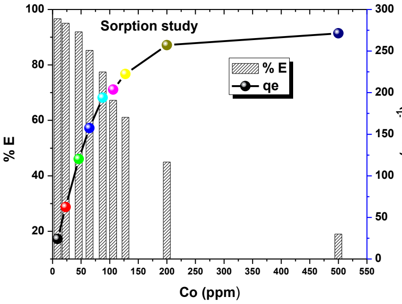

Figure 2. U sorption study with APAN-alginate beads

Polymer-based composites, including beads, films, membranes, fibres, and nanocomposites, have emerged as promising materials for uranium removal due to their stability, versatility, and low cost, making them ideal for solid-phase extraction of radionuclides. The present work has been focused on the radiation-induced synthesis of provide its expaned form (PAN), their modification and synthesis of Amixoximated APAN-alginate beads (APAN-Alg beads) (Figure 1), for sorption of uranium from aqueous waste. These beads were characterized using SEM, TGA-DSC and FT-IR to determined their composition and morphology. The synthesized APAN alginate beads were evaluated, for their ability to adsorb uranium from aqueous solution, at varying uranium concentrations, different temperatures and pH values. The kinetic measurement showed that about 180 min of equilibration time was enough, to remove saturation amount of uranium. The uranium uptake capacity of the polymeric beads was found to be very high ~200 mg/g of the dry beads, as shown in Figure 2.

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RC - 6

EFFECT OF GAMMA IRRADIATION ON WHOLE MACKEREL FISH

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Gamma irradiation is a known and commonly used fish preservation method that does not cause any increase in temperature, decreases the microbial population, and extends fish shelf life [1]. Present study focused on the impact of γ-radiation on the nutrient, sensory attributes, microbial quality, biochemical properties of fresh whole mackerel fish and its shelf-life extension. Fish was packed in polypropylene package and irradiated at 2 kGy dose. The proximate, microbial load, sensory quality and fatty acid composition of whole mackerel fish on storage at 1°C was studied. The results indicated no significant changes in proximate content, sensory, biochemical quality and fatty acid composition. The moisture, protein, fat and ash contents were 75.28 ± 1.49, 13.49 ± 0.19, 9.28 ± 0.85 and 1.95 ± 0.02 respectively. The bacterial load of 4.25 log CFU/g was reduced to 2.04 log CFU/g and total mold count reduced from 1.17 log CFU/g to below detection limit at 2 kGy. The fatty acid composition of control and treated samples were in the range 51.36±2.63, 16.35±.0.77 and 32.29±2.9 % for saturated (SFA), monounsaturated (MUFA) and polyunsaturated (PUFA) fatty acids respectively. The control sample was spoiled on 7th day of storage with bacterial count of 6±0.1 log CFU/g and total mold count of 2.7±0.06 log CFU/g. Irradiated samples were acceptable up to 15th day of storage and spoiled on 18th day with total bacterial load of 6.2±0.4 log CFU/g. Hence, the results suggest radiation dose of whole Mackerel at a dose of 2 kGy extends the shelf-life by improving microbial safety with no effect in sensory and nutritional qualities.

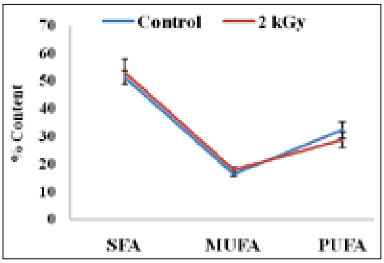

Figure 1: Fatty acid composition of whole mackerel fish

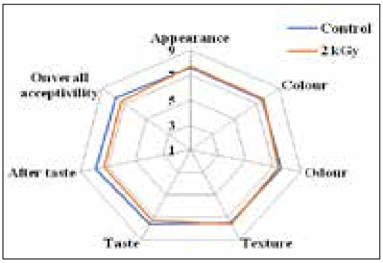

Figure 2: Sensory analysis

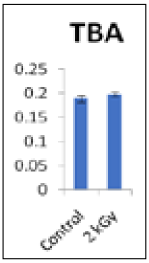

Figure 3: Biochemical analysis

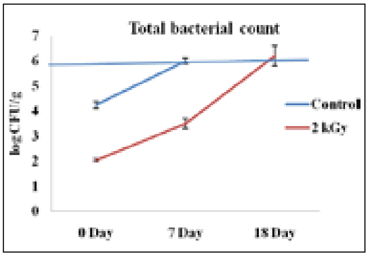

Figure 4: Microbial analysis on storage

Reference

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RC - 7

SYNTHESIS OF PLASTIC SCINTILLATOR LOADED WITH GADOLINIUM OXIDE NANOCRYSTAL

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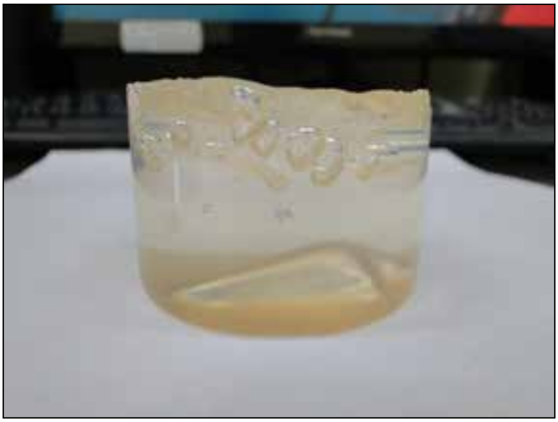

Figure 1: Photograph of Gadolinium nanocrystal loaded Plastic scintillator.

Heavy element loaded plastic scintillation detectors have been proposed to detect high energy X-rays and gamma rays. Plastic scintillators provide the advantage of large area/large sized detectors and high Z allows better photoelectric effect. But these kind of high Z element loaded polymer composite suffers from diminished light output resulting from fluorescence quenching and opacity [1].

We demonstrate the synthesis of transparent plastic scintillator loaded with Gadolinium which has comparable light output as commercially avalaible plastic scintillator. Gd loaded plastic scintillator with 5 cm diameter and 2.5 cm thickness was synthesized and 0.1 wt% Gd loading could be achieved.

BMEP capped Gadolinium oxide nanocrystals (Gd-BMEP) were synthesized by thermal decomposition method. Gd-BMEP was then polymerised with styrene to get the Gadolinium loaded plastic scintillator.

The plastic scintillator can be used for gamma ray detection with with higher probablity of photoelectric effect and higher sensitivity. It can also be used for the detection of thermal neutrons via thermal neutron induced reaction, since Gd-155 and Gd-157 has the highest thermal neutron crossection among the naturally occuring elements.

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RC - 8

ENHANCED RADIOLYTIC DEGRADATION OF METHYLENE BLUE DYE WITH MXENE

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Introduction: The treatment of textile effluents which contain dyes and other refractory pollutants becomes difficult and need additional treatment technologies to accelerate the degradation of pollutants [1]. Hence the needs of innovative hybrid techniques are required. Ionizing radiation presents a promising method for treating textile effluents, largely because its effectiveness can be enhanced in aqueous solutions through the primary products generated from water radiolysis [2].

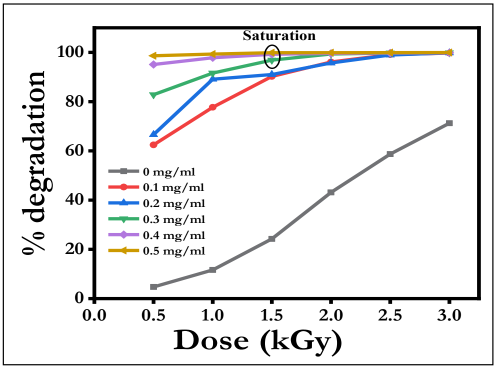

Figure 1. Degradation of Methylene blue dye under gamma radiation with different concentrations of Mxene.

Result and Discussion: In this study, gamma radiation was employed to degrade methylene blue (MB) dye, and Mxene (100µm) used as catalysts to improve degradation efficiency. 50 ppm dye solution was prepared using DI water and different concentration (0.1 to 0.5 mg/ml) of Mxene-100 (100µm size) suspension was added as a catalyst. The solution of dye and Mxene was irradiated using gamma radiation with different absorbed doses, 0.5 to 3.0 kGy. Then the solution is centrifuged for the complete removal of the catalyst. The irradiated solution was subsequently used for absorption studies on a spectrophotometer after each irradiation.

It is evident from graph that the dye solution containing Mxene shows better degradation percentage than the solution without Mxene-100. Also with increase in the concentration of Mxene, the extent of degradation of methylene blue also increases due to its fast charge carrier separation and high surface area. After a certain concentration of Mxene-100 (0.3mg/ml) and dose 1.5kGy, saturation in degradation (about 98% degradation) is reached leading to very minimal change of degradation percentage.

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RC - 9

COBALT COMPLEX FOR HYDROGEN EVOLUTION REACTION IN AQUEOUS MEDIUM

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Hydrogen is regarded as potential fuel for clean energy applications [1]. Cobalt is well known metal for the catalysis of hydrogen evolution reaction [2]. Herein, cobalt complex with iminodiacetate (IDA) ligand has been prepared in aqueous solution and extracted as single crystal from the solution. The single crystal XRD data showed that the cobalt centre is bonded with two IDA ligands. The NMR and FTIR data also supports the complexation. The electrocatalytichydrogen generation was studied in aqueous medium on glassy carbon electrode. The complex showed increase in cathodic current compare to the blank after -1.3 V due to hydrogen evolution reaction. Deposition of cobalt nanoparticles onto glassy carbon was observed due to reduction of complex. The hydrogen generation was observed due to the catalysis of both complex as well as cobalt nanoparticles. The tafel slope was found to be 68 mVs/dec, implies Volmer-Heyrovsky mechanism. For further investigation, pulse radiolysis has been carried out in aqueous solution at different trifluoroacetic acid (TFA) medium. The complex showed high obsorption at 383 nm. With increasing TFA concentration, the decay of the absorbance at 383 nm became faster indicating catalytic activity of the complex.

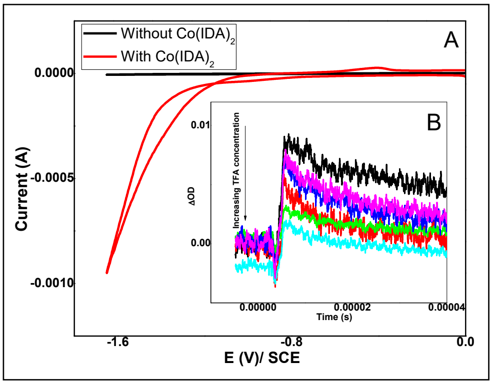

Figure 1. A) Cyclic voltammogram with and without cobalt complex in 1 M PBS at pH 7. B) Pulse radiolysis of cobalt complex at different TFA concentration.

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RC - 10

EXPERIMENTAL L- SHELL X-RAY RELATIVE INTENSITIES OF ^{83}Bi INDUCED BY HIGH-ENERGY B^{q+} IONS

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In this paper, we present the relative intensities for different L- shell X-ray lines in ^{83}Bi, induced by bombardment with 30 and 45 MeV B^{q+} (q=3,4) ions. The measurements were carried out at the 16UD Pelletron Accelerator at the Inter-University Accelerator Centre (IUAC) in Delhi. Thin targets, evaporated onto ultrapure carbon backings of thickness ~20 μg/cm^2, were bombarded by boron ions. These targets were mounted on a steel ladder and positioned at 45° angles to both the beam direction and the SDD detector within an evacuated ($<10^{-6}$ Torr) scattering chamber. The L- X-ray spectra were deconvoluted using computer code ORIGIN, after subtracting the background spectra recorded using blank carbon as target at each incident ion energy. Experimental results were compared with theoretical values calculated using the ECPSSR model [1] for ion-induced sub-shell ionization cross-sections, the Dirac-Hartree-Slater (DHS) model [2] for X-ray emission rates, and fluorescence and Coster-Kronig yield data from the DHS model [3]. The observed discrepancies between measured and calculated values may be attributed to multiple ionization effects induced by the incident boron ions. These results enhance our understanding of atomic interactions in ion-beam-induced X-ray emission and offer valuable insights for materials science and nuclear physics applications.

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RC - 11

RADIATION CHEMICAL STUDIES OF THIOFLAVIN T (ThT): AN UNEXPLORED AREA OF RESEARCH

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Thioflavin T (ThT) is a popular dye for its dramatic changes in its fluorescence properties on interaction with amyloid fibrils. It consists of a dimethylated benzothiazole ring linked to a dimethylamino benzyl ring through a carbon–carbon single bond. It was observed that the sensitivity of amyloid detection by ThT is very much dependent on the purity of the compound. In case of photoirradiation there was partial conversion of ThT into oxidized and demethylated derivatives [1]. To understand the redox behaviour of ThT, radiation chemical reaction was carried out using steady state and time resolved methods. Time resolved studies were carried out in 7 MeV electron accelerator-based pulse radiolysis setup and for steady state irradiation Cobalt-60 gamma chamber (GC-1200) was used. The ${}^{\bullet}$OH radical reaction of ThT at neutral pH resulted transients that have absorption band at 330 and 480 nm as observed in pulse radiolysis studies (Figure 1 A). Steady state gamma irradiation of ThT resulted decrease in the absorbance at 412 nm with increasing absorbed dose. Interestingly, there was a blue shift in the absorption maximum of ThT and appearance of a shoulder at 470 nm with increase in absorbed dose. When absorbed dose of 23 Gy was used for 50 µM of ThT under ${}^{\bullet}$OH radical reaction condition it was observed that the most of the ${}^{\bullet}$OH radicals react with ThT. The degraded products of ThT can be dihydroxylated and/or trihydroxylated ThT in the benzothiazole moiety. Hydrated electrons (e^-_{aq}) also are one of the primary radiolytic products of water. The transient product for e^-_{aq} reaction with ThT have absorption maxima at 370 nm at pH 7 (Figure 1 B). The appearance of absorption band at 370 nm is a consequence of e^-_{aq} adduct formation at the cationic imine bond of ThT.

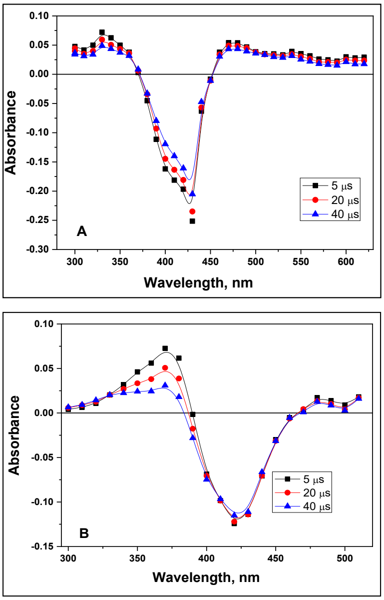

Figure 1. Transient absorption spectra for the reaction of ${}^{\bullet}$OH radical (A) and e^-_{aq} (B) with 50 µM of ThT at pH 7. The legend refers to the signal recording time after delivery of the electron pulses. Dose per pulse 18-20 Gy.

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RC - 12

RADIATION INDUCED SYNTHESIS OF GOLD NANOPARTICLE DECORATED GLYCOPOLYMERS FOR ANTICANCER DRUG DELIVERY

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The use of gold compounds as therapeutics, has been recognized as one of the oldest forms of medicinal treatment of physiological ailments, such as rheumatoid arthritis and psoriasis, due to its unique anti-inflammatory properties. Interestingly, engineered gold nanoparticles (AuNP) display an extraordinary combination of chemical inertness, surface modifiable substrate, and size/shape-dependent optical properties, which makes them ideal candidates in biomedical applications. Carbohydrate-based anticancer agents have been explored with the aim of increasing the efficacy and decreasing the side effects of traditional anticancer drugs[1].

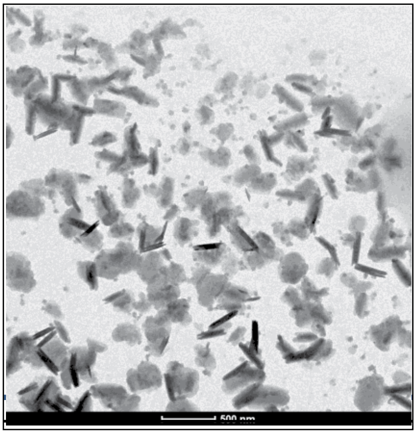

Figure 1. HRTEM image of self-assembled glycopolymer synthesized by gamma radiation induced polymerization

Glycopolymers were synthesized with different sugar functionalities like glucose, galactose and mannose by gamma radiation induced polymerization[2]. The effect of absorbed dose on the structure and properties of the synthesized polymers were investigated. The self-assembled polymers had a zeta potential of -11 mV where as the unirradiated monomer solution had near neutral zeta potential.

The morphology of the glycopolymers were studied using HRTEM images, which revealed interconnected fibrillar assemblies. AuNPs were also generated insitu by gamma radiation the formation of which was confirmed by UV-Vis spectroscopy. These polymers were loaded with model anticancer drug Doxorubicin electrostatically which later on exhibited pH dependent release profile.

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RC - 13

RADIOLYTICALLY SYNTHESIZED SILICA NANOPARTICLES AS A ROBUST FLUOROPROBE FOR SENSING OF Cr (VI): PAPER STRIP-BASED DETECTION AND ANTIOXIDANTS PROPERTIES

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Silica nanoparticles (SiO_2 NPs) have emerged as versatile materials with wide-ranging applications in various fields, such as biomedical imaging, environmental sensing, catalysis, and optoelectronics[1]. Considering their imminent importance, a highly rapid, eco-friendly, and one-pot scalable approach based on radiation-induced technique is being reported for their preparation[2,3].

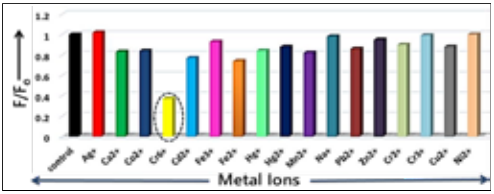

Figure 1. Effect of various metal ions on the PL of CD@ SiO_2 NPs.

Electron-beam was used to derive the formation of SiO_2 NPs, while *in situ* functionalization was carried out by a-Cyclodextrin (a-CD). The as obtained a-CD functionalized SiO_2 NPs (CD@ SiO_2 NPs) were photoluminescent. Notably, the NPs photoluminescence (PL) could be tuned from blue to green with the increase in the imparted dose[3]. Nonetheless, we could selectively enhance blue PL multifold times over green PL. This aspect was explored for the highly selective sensing of Cr (VI) ions, a well-known environmental hazard. Figure 1 shows the plot of F/F_0 versus metal ions. As can be seen, CD@SiO_2 NPs exhibited remarkable effectiveness in the trace level detection of Cr (VI) ions. Mechanistic studies revealed inner filter effect (IFE) based PL quenching. Furthermore, to assess the practicality of real-time detection, paper strips have been developed with cellulose incorporated powder of as prepared CD@SiO_2 NPs for visible detection of Cr (VI) ions using a handheld UV lamp. Additionally, antioxidant properties of CD@SiO_2 NPs were evaluated using ABTS & DPPH protocols, revealing significant radical scavenging efficiency. All these findings will be presented in detail.

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RC - 14

INVESTIGATION OF RADIOLYTIC FORMATION OF VO$_2$ NANOPARTICLES VIA ALCOHOL RADICALS

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Vanadium dioxide (VO$_2$) is considered as one of the smart materials which exhibits thermochromic behaviour, metal (tetragonal rutile phase at lower temperature) to insulator (monoclinic phase at higher temperature) transition at critical temperature Tc 68℃ [1]. It reflects IR radiation above Tc and transmits IR radiation below Tc making it a suitable candidate for smart window material.

Vanadium oxide was synthesized using sodium metavanadate (NaVO$_3$) as the precursor, via radiation chemical method. Sample solutions were irradiated with electron pulses of FWHM 2ms in a 7MeV LINAC. 2-Propanol (IP), n-propanol (n-POH), ethanol (EtOH) was used for the generation of alcohol radicals, which are reducing in nature and required for the synthesis.

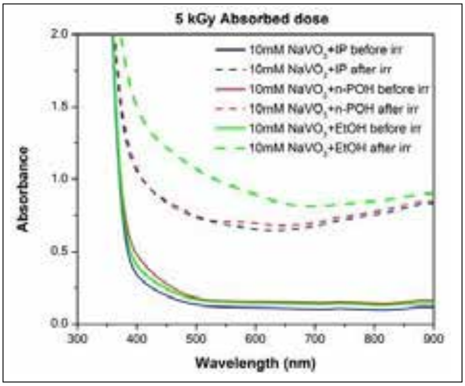

Figure 1. Absorption spectra recorded for a reaction mixture containing 10mM NaVO$_3$ and three different alcohols before (solid) and after (dotted) 7 MeV electron beam irradiation.

Water radiolysis produces three major free radicals, e_{aq}^-, $H^\bullet$ and $^\bullet OH$, out of which OH radicals are oxidising and rest two are reducing. Alcohols react with $H^\bullet$ and $^\bullet OH$ radicals to produce corresponding C-centred alcohol radicals, which are reducing in nature [2]. Therefore, under N$_2$O saturated condition, only alcohol radicals would be generated and these will react with VO$_3^-$ to initially form an intermediate species and then VO$_2$ in a de-aerated condition in the aqueous-alcohol solution. Subsequently, these VO$_2$ will undergo nucleation and growth to form VO$_2$ nanoparticles, which are substantially stable in the absence of air. The formation of such intermediate species was investigated through the pulse radiolysis studies under various experimental conditions. One reaction pathway in the case of ethanol is shown below.

$$CH_3C^\bullet HOH + VO_3^- \longrightarrow [CH_3C^\bullet HOH{:}VO_3] \longrightarrow VO_2 + CH_3CHO + OH^- \qquad (1)$$

It is expected that this method of synthesis is very effective and does not require any additional reducing agents as well as no hazardous chemical load on the environment.

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Photochemistry Posters (PC)

PC - 1

DESIGN AND SYNTHESIS OF pH-RESPONSIVE, WATER-DISPERSIBLE N,S-DOPED RED EMISSIVE CARBON DOTS FOR BACTERIAL IMAGING

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Carbon dots (CDs), fluorescent carbon nanoparticles smaller than 10 nm, have been extensively used in sensors, bioimaging, catalysis, light-emitting (LEDs), and photoelectronic devices [1]. This is due to their unique characteristics, including low toxicity, biocompatibility, high photostability, ease of surface modification, and up-conversion fluorescence. Carbon dots (CDs) have proven effective in revealing the 3D structures of biological samples, distinguishing between normal and cancer cells, and detecting various analytes inside cells [2]. Most of the carbon dots are blue-green emitting CDs. The practical use of blue-green-emitting carbon dots (CDs) is limited by their shallow penetration, photobleaching, and autofluorescence issues [3]. The synthesis of red-emissive carbon dots (CDs) is highly sought after for sensing applications, but challenges remain in precursor preparation and product purification. Red-emissive carbon dots (RCDs) have been developed to address these issues. RCDs offer deep tissue penetration, reduced photodamage, low autofluorescence, and high imaging contrast. Herein, we designed and synthesized RCDs with high water dispersibility, low toxicity, and excellent optical properties using the hydrothermal method. These features make them ideal for a range of biological applications.

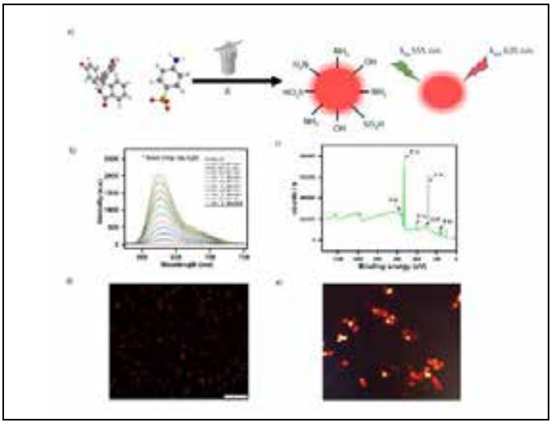

Figure 1. a) Graphical representation of synthesis of CDs. b) Fluorescence response of R-CDs in water. c) XPS data of the R-CDs d) E. coli staining using CDs e) S. aureus staining using CDs.

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PC - 2

HALOARENE-DERIVED MULTIFUNCTIONAL AMIDES AND SULPHONAMIDES AS POTENTIAL DRUG CANDIDATES

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Amides are present in many intriguing substances, including proteins, pharmaceuticals, and alkaloids, making them one of the most significant functional groups in organic chemistry. The amide group’s exceptional capacity to create pertinent hydrogen bonding interactions has attracted a lot of interest. The carbonyl (>C=O) and amido (-NH-) groups of an amide can function as hydrogen bond donors or acceptors, respectively. Similarly, sulphonamide is a well-known functional group present in many antibiotics, such as sulpha drugs. In literature, many sulphonamide-containing compounds have been utilized as hypoglycaemic agents, anticancer agents, carbonic anhydrase inhibitors, etc. Furthermore, halogen atoms are commonly present in organic molecules, and halogen functionalization is of great significance in organic synthesis to achieve the desired material and biological functions. In crystal engineering, the halogen bond is an intriguing interaction utilized to design molecular solids. Combining the concepts of amides and sulphonamides with the impact of halogen in the area of pharmaceuticals and structural engineering, we herein propose a series of multi-functionalized, halogen-containing tertiary amides and sulphonamides by an easy two-step synthetic methodology. The synthesized molecules were characterized by different spectroscopic and spectrometric analyses, and structural elucidation was done by Single-crystal X-ray diffraction studies (figure 1). These new molecules have the potential to be used in medication development and material sciences, underscoring its importance for current investigations in both domains.

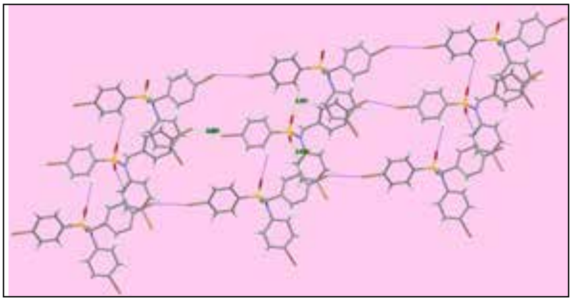

Figure 1. Infinite chain of hydrogen and halogen bonding in a sulphonamide derivative

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PC - 3

SUPRAMOLECULAR HOST-GUEST COMPLEXATION OF AMPHIPHILIC STYRYL DYES WITH CYCLODEXTRIN DERIVATIVES

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Amphiphilic fluorescent organic dyes are known to form self-assemblies in aqueous solution leading to modulation in their photophysical properties [1]. This work demonstrates synthesis of three novel amphiphilic styryl dyes with varying length of alkoxy side chains ($C_{18}H_{37}O$-, $C_{10}H_{21}O$-, and CH_3O-) and tuning of their aggregation behaviour via supramolecular host-guest complexation.

The monomeric form of all the dyes show emission centered at 505 nm whereas the aggregates show a broad peak around 620 nm in aqueous solution. Tuning of aggregation behaviour of the dyes were demonstrated by supramolecular complexation with Sulfobutylether-b-cyclodextrin ($SBE_7\beta$-CD) and β-cyclodextrin (β-CD) [2]. The dodecyloxy ($C_{18}H_{37}O$-) derivative shows aggregation with large enhancement in the fluorescence yield (~4 fold enhancement) at smaller concentrations of $SBE_7\beta$-CD, while at higher concentrations monomeric peak gets regenerated. Furthermore, complexation with β-CD leads to no such enhancement in the fluorescence intensity at lower concentrations, while monomeric peak is still regenerated at higher concentrations of host. Depending on the chain lengths, other dyes exhibit differential aggregation and deaggregation behaviour upon interaction with $SBE_7\beta$-CD and β-CD. The large Stokes shift upon aggregation can be further utilized for ratiometric sensing of analytes.

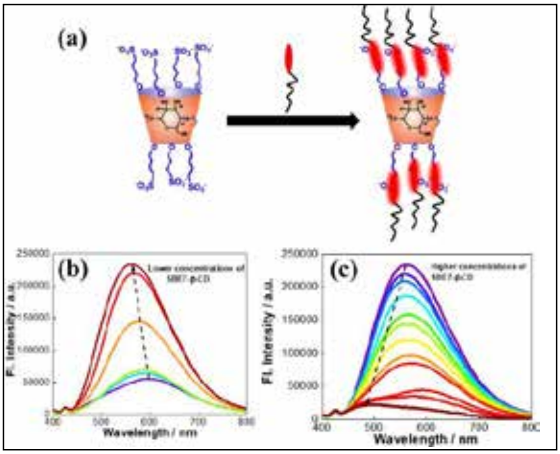

Figure 1. (a) Schematic for aggregation of amphiphilic styryl dyes at $SBE_7\beta$-CD portals. Emission change of dodecyloxy derivative (b) at lower $SBE_7\beta$-CD concentrations (c) at higher $SBE_7\beta$-CD concentrations.

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PC - 4

DICARBATRIPHYRIN(2.1.1) AND ITS CARBACALIX[1]PHYRIN ANALOGUE: STRUCTURE- PROPERTY RELATIONSHIP AND APPLICATION AS A Fe(III) CHEMOSENSOR

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Triphyrins are contracted porphyrins with three pyrrole rings in its macrocyclic framework. By introducing phenyl units inside the triphyrin core, carbatriphyrins can be synthesized as an integral component of the macrocyclic structure. Insertion of phenyl groups in the core contributes distinctive characteristics to carbocyclic reactivity,and formation of organometallic complexes.[1] The arrangement of phenyl ring(s) within the macrocyclic framework is crucial in defining their attributes, especially in distinguishing the behaviors of ortho-, meta-, and para-phenyleneswhen incorporated into either macrocycle [2] or oligophenylene architectures.[3] The carbatriphyrins that have been documented so far have been exclusively in their protonated form or as organophosphorous,i.e. P(V) complex. In this poster, we wish to present the synthesis and characterization of a newly developed stable dicarbatriphyrin (2.1.1) (**C**), achieved by modifying the [14]triphyrin(2.1.1) (**A**) framework. Furthermore, the synthesis of carbacalix[1]phyrin(2.*1.1*) (**B**), a phlorin analogue of dicarbatriphyrin (2.1.1), reveals a chair conformation in contrast to the saddle-shaped structure of its oxidized variant. The dicarbatriphyrin (2.1.1) displays fluorescent emissionin solution, which is specifically quenched by Fe(III) ions, underscoring its potential utility as a chemo-sensor for Fe(III) cations.

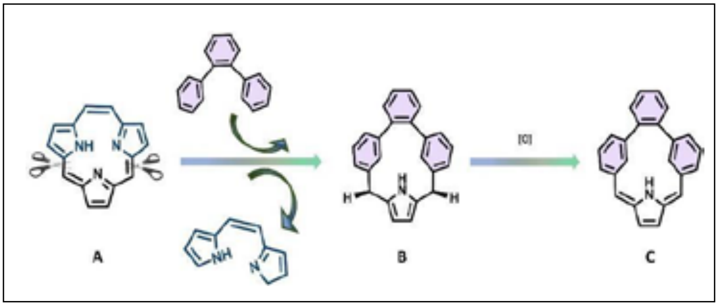

*Figure 1: Incorporation of polyphenylene unit in the triphyrincore (**A**) to achieve carbacalix[1]phyrin(**2**.1.1 (**B**) and itsoxidized form dicarbatriphyrin(2.1.1)(**C**).*

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HOW PEG-BASED CROWDERS AFFECT ULTRAFAST ENERGY FLOW IN HEME PROTEINS

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The study of energy flow in proteins, though very complicated to track at the molecular level, is crucial for understanding how proteins function [1]. The dimension of a protein molecule and its vibrational density of states havea significantimpact on the diffusion of energy in protein,affecting thetimescale of diffusion.Hence energy exchange between numerous vibrational degrees of freedom, i.e., vibrational energy flow/transfer (VET), is an important mechanism by which a protein keeps its temperature relatively constant while performing intracellular processes. Amongst the proteins that have been fairly well studied are theheme proteins (e.g., cytochrome *c,* myoglobin) [2,3]. Cytochrome *c* (cyt c) is an important electron transport redox protein inside mitochondria while myoglobin (Mb) is primarily responsible for oxygen storage in muscle tissues.Heme cofactor is not only a good photo-thermal converter, but also undergoes ultrafast energy dissipation, upon photoexcitation over a range of wavelengths. This aspect has been captured using femtosecond transient absorption spectroscopy thereby providing vital information about the factors affecting energy flow in heme proteins. Cyt*c* has a 6-coordinated iron centre in heme that is buried, while myoglobin has a penta-coordinated Fe in heme cofactor that is comparatively exposed. Using ultrafast transient absorption spectroscopy we have compared the effects of PEG-based crowders of different molecular weights on the energy flow in cyt*c* and Mb. Among the four and three decay channels observed globally in cyt*c* and Mb respectively, the longest component (through space energy transfer) was severely affected by the crowding environmentsincyt*c*as in PEG 8 $\boldsymbol{\tau}_4$ was very long whereas the longest component was less affected for deoxy Mb in different PEGs.

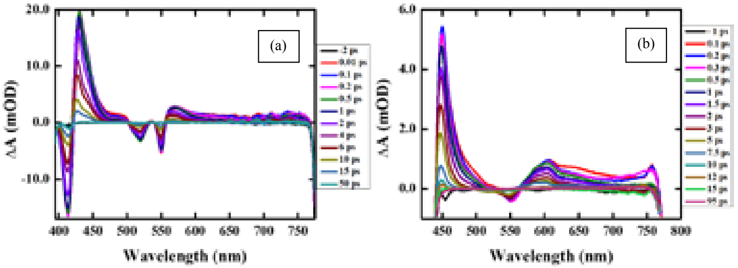

Figure 1. Transient absorption spectra of (a) ferrous cyt c and (b) deoxy Mb in PEG 1 of 50g/L (l_{pump}= 400nm).

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PHOTOPHYSICAL STUDY OF A BENZOTHIAZOLE DERIVATIVE AND ITS INTERACTION WITH CYCLODEXTRIN HOSTS

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Benzothiazole derivatives show potential as imaging probes and anticancer agents due to their ability to target specific sites and produce strong fluorescence signal. However, their poor water solubility often limits their bioavailability. This can be overcome through encapsulation by host molecules. In this work, we examined TEG-BTA-2, a derivative that combines the benzothiazole unit (BTA-2) with a neutral, non-toxic tetraethylene glycol unit (TEG), for improved diffusibility [1]. We investigated the photophysics of TEG-BTA-2 in various solvents (water, acetonitrile, methanol, ethyl acetate). The absorption and emission spectra exhibited slight red shift with increase in solvent polarity. The emission maxima were 441 nm in water and 411 nm in ethyl acetate. The highest fluorescence quantum yield was observed in acetonitrile (QY=0.53). Additionally, we investigated the pH-dependent behavior of TEG-BTA-2 in aqueous solutions, revealing two emissive species in the monoprotonated form and one in the diprotonated form. Cyclodextrins (CDs) were used to study host-guest complex formation with TEG-BTA-2 [2]. We found significant changes in fluorescence yield, lifetime, and spectral characteristics of TEG-BTA-2 due to the formation of 1:1 and 1:2 host-guest complexes with β-CD and γ-CD, respectively. Interestingly, complex formation with β-CD led to increase in fluorescence intensity while complex formation with γ-CD led to decrease in fluorescence intensity. The study underscores the selective binding of cyclodextrins and their potential to optimize the dye's fluorescence properties through supramolecular interactions.

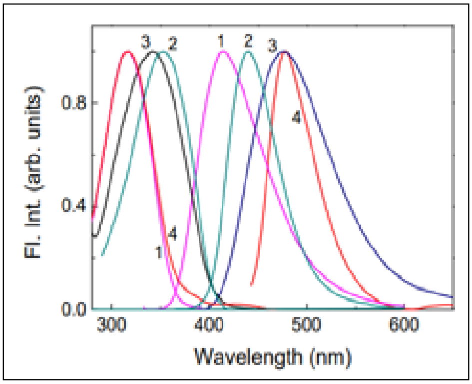

Figure 1. Comparative study on normalized emission and corresponding excitation spectra of TEG-BTA-2 in aqueous solution of (1) Monoprotonated form (pH 1.17), 323 nm excitation and 414 nm emission, (2) Neutral form, 350 nm excitation and 430 nm emission, (3) Di protonated form (H_0 -1.4), 346 nm excitation and 476 nm emission and (4) Monoprotonated form (pH 1.17), 428 nm excitation and 478 nm emission.

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N-HETEROCYCLIC RESORCIN [4] ARENE CAVITANDS: A VERSATILE PLATFORM FOR DIFFERENT APPLICATIONS

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Resorcin[4]arenes are the unique class of supramolecular building blocks generally prepared by the acid catalyzed condensation reaction of resorcinol and aldehydes. Resorcin[4]arenes are known for their well-defined cyclic tetrameric cavity with rich π-electron environment. Easy substitutions at the upper rim, lower rim and their multiple hydroxyl (-OH) groups provides a greater scope for the synthetic manipulation for the generation of new class of resorcin[4]arene cavitands and their applications in host-guest chemistry, nanoscience, catalysis, medicinal chemistry. Installation of heterocyclic moieties into the cavitand system increases its potential and provide more scope of applications. Since many years' pyridine derivatives are found to be an excellent stabilizer to gold nanoparticles. In the present work two different type of water soluble resorcin[4]arenes having hydrophilic 2- and 4- pyridinyl groups at feet-regions have been synthesized and their applications as both reducing and stabilizing agent for the synthesis of stable gold nanoparticles has been extensively studied. Water soluble tetrakis(4-pyridinyl) resorcin[4]arene cavitand shows pH sensing ability due to presence of both donor (hydroxyl) and acceptor (pyridine) groups. The real time pH sensing application has been carried out through naked eye colorimetric experiment using both solution phase and C-4-pyridyl resorcin[4]arene based pH paper. A colour change from orange to pink is observed in basic medium. It is also observed that supramolecular host molecules such as calixarenes, cyclodextrins, pillararenes, cucurbiturils etc show better receptor properties and have been used as a potential candidate in the drug delivery field. Thus owing to the water solubility behaviour of resorcinarene based cavitand molecules along with pH responsive characteristic, it may be further explored for their promising application in the field of host guest chemistry pertaining to the drug delivery.

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KINETIC INVESTIGATION OF BUTYLAMINE WITH OH RADICALS

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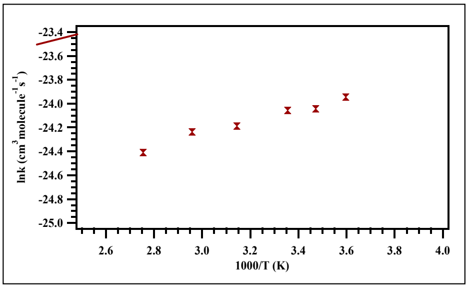

Figure 1. Arrhenius plot for the reaction of butylamine with OH radicals in the temperature range of 278-363 K. The fragmented lines designate a linear fit and the vertical error bars in data points are in 2σ

The chemistry of the Earth's atmosphere is highly complex, involving countless chemical species that exist in various phases and over wide ranges of temperature and pressure. Research in atmospheric chemistry often focuses on gas-phase reactions, particularly the oxidation of volatile organic compounds (VOCs). The oxidation of VOCs is primarily initiated by the hydroxyl (OH) radical, which is formed in presence of sunlight, but it also involves reactions with other oxidants[1]. Amines are extensively used in the pharmaceutical industry and in developing chemicals for crop protection, medication, cleaning products, petroleum, and water purification.To date, approximately 150 amines have been identified in the atmosphere. The most common and abundant amines are low-molecular-weight aliphatic amines with carbon numbers of 1−6, which are highly volatile. Amines likebutylamine are emittedinto the atmosphere from natural sources like oceans, biomass burning, vegetation, and geological activities[2]. The kinetic study of butylamine with OH radicals was performed using Pulsed Laser Photolysis-Laser Induced Fluorescence (PLP-LIF). in the 278 – 363 K temperature range. A double-jacketed pyrex cell was used to maintain the temperature of the reaction. In this technique, a Kr Fexcimer laser lasing at λ = 248 nm was used for photolysis of precursor H_2O_2. Nd:YAG pumped dye laser at 281.9 nm was used as a probe laser, and a photomultiplier tube was used to detect the fluorescence at 308 nm. These three were placed atorthogonal to each other. The laser beams enter the reaction cell through the window at a Brewster angle. The rate coefficients for the reaction of butylamine with OH radicals show a negative temperature dependence over the temperature range of 278 – 363 K.

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SYNTHESIS AND BIOLOGICAL EVALUATION OF FLUORESCENT BENZOISOQUINOLONYL PEPTIDE/ TRIAZOLE CONJUGATED β-D-RIBOFURANOSE

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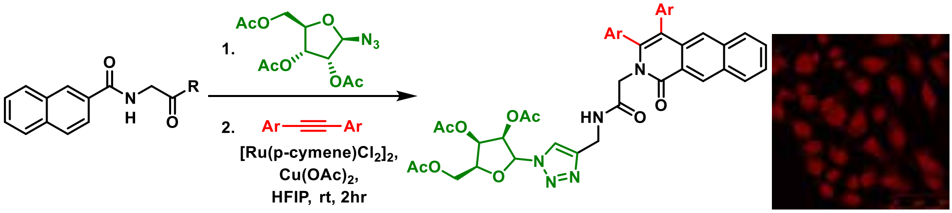
Isoquinolone and its derivatives are N-heterocyclic aromatic molecules, which are constituents of various alkaloid natural products possessing a wide range of pharmacological and physiological activities[1,2]. Benzoisoquinolone is one such aryl extended derivatives of isoquinolones. This report describes conjugation of benzoisoquinolonyl peptide derivatives with **β**-D-ribofuranose along with a triazole linker utilizing Cu-catalysed cycloaddition. It has beenthen subjected to Ru-catalysed C(sp^2)–H activation annulation at room temperature[3]. The amide *N*-terminal functions as an intrinsic directing group, coordinating with the active Ru(II) catalyst to facilitate C–H bond activation resulting in fluorescent **β**-D-ribofuranose conjugated benzoisoquinolonyl peptide hybrid. Significantly, cell proliferation assay depicts no significant cytotoxicity to normal human Hek-293T and cancerous HeLa cell lines. They also depictedreasonably high quantum yield of ~36% along with good cell permeability into HeLa cell nucleus. Hence, we have successfully synthesized fluorescent and cell permeable benzoisoquinolonyl peptide and triazole linked **β**-D-ribofuranose derivative utilizing Cu-catalysed cycloaddition and late stage Ru-catalysed C(sp^2)–H activation.



- Cu-catalysed cycloaddition
- Late stage Ru-catalysed C(sp^2)-H activation
- ~36% Quantum Yield
- Good cell permeability into HeLa cell nucleus

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ULTRAFAST DYNAMICS OF NONRIGID NICKEL PORPHYRIN DIMER

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Photosynthesis is a vital process in nature for sustaining life. The photosynthetic reaction center consists of two bacteriochlorophyll molecules, known as 'Special Pair' [1]. Photophysical properties of these molecular dimers strongly depend on different structural factors e.g. the constituent chromophores, linkage position, dihedral angle, and centre-to-centre distance. Here, photophysical properties of ethane-bridged Nickel octa ethyl porphyrin dimer has been explored and compared with its monomer analogue, an attempt to understand the behaviour of the 'Special Pair'. The ethane bridge links the two porphyrin units, potentially affecting their electronic coupling and altering the excited-state dynamics. Using Ultrafast Transient Absorption Spectroscopy, the excited-state lifetimes and relaxation dynamics of these systems have been explored. The results reveal significant differences in the excited-state dynamics between the monomer and dimer. Initial photoexcitation is delocalized over the porphyrin π ring. However, intramolecular vibrational relaxation is hampered by intermediate states involving metal d orbitals [2]. Excitonically coupled porphyrin dimer causes an ultrafast deactivation, unlike the monomer. Axial ligand binding plays a role in vibrational relaxation pathways that give us a better understanding of excess energy dissipation of highly excited Nickel (II) porphyrins into surrounding solvent molecules.

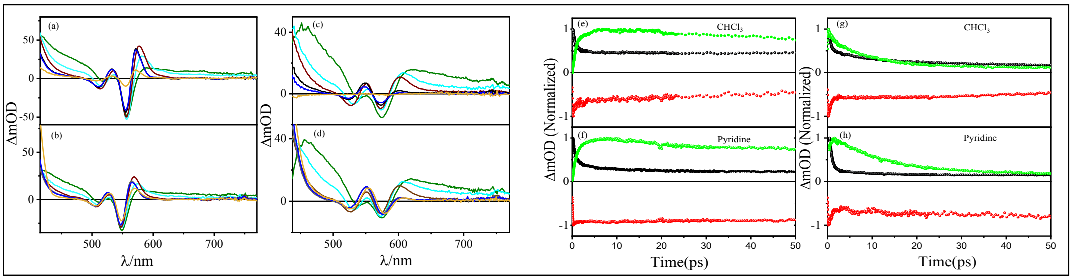

Figure 1. (a) and (b) TA spectra of Ni porphyrin monomer in chloroform and pyridine respectively. (c) and (d) TA spectra of Ni porphyrin dimer in chloroform and pyridine respectively with λ_{pump} = 400 nm. (e) and (f) Kinetics of GSB (red) at 550 nm, ESA (green, black) signal at 450 nm, 565 nm of monomer in chloroform and pyridine respectively. (g) and (h) Kinetics of GSB (red) at 575 nm, ESA (green, black) signal at 470 nm, 600 nm of dimer in chloroform and pyridine respectively.

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FÖRSTER RESONANCE ENERGY TRANSFER FROM PYREDIYNE QUANTUM DOTS IN GEL MEDIA

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Förster resonance energy transfer (FRET) is a non-radiative, short-range transfer of emissive energy of the donor to an acceptor. The distance dependent nature of FRET had been exploited extensively to probe various micro heterogeneous environments and to study interactions between biomolecules [1]. However, narrow spectral coverage, rapid photo bleaching and quenching due to excimer formation limits the applications of organic dyes as FRET donors. When compared to organic dyes, semiconductor quantum dots have broad absorption spectrum, high molar extinction coefficient, better photo stability and high surface to charge ratio which aids in bio conjugation [2]. Nevertheless, traditional semi-conductor quantum dots suffer from blinking effect and cytotoxicity. To address these issues, pyrediyne quantum dots (PDYQDs), which have negligible cytotoxicity, good spectral coverage and significant photoluminescence quantum yield have been selected as FRET donor [3]. Thus, in the current study PDYQDs (Fig. 1a) were synthesized following a literature protocol, characterized using UV-visible absorption spectroscopy (Fig.1c) and transmission electron microscopy (TEM) imaging technique [3]. To test the applicability of PDYQDs as a FRET probe in micro-heterogeneous environments, FRET from PDYQDs to various organic dyes were analysed in leucine based organogel (OG-leucine) (Fig. 1b). As shown in fig. 1d and e, the excitation dependent emission behaviour and the longer wavelength emission peaks of PDYQDs observed in ethanol were lost upon incorporation into gel medium. Furthermore, the emission behaviour of PDYQDs in gel media was analogous to the emission spectra of PDYQDs in toluene (Figure 1f), which indicated that the QDs resides in the toluene pool of the gel medium. Thus, maximum FRET efficiency from PDYQDs to organic dyes was observed for organic dyes that resides in the toluene pool and are non-polar in nature.

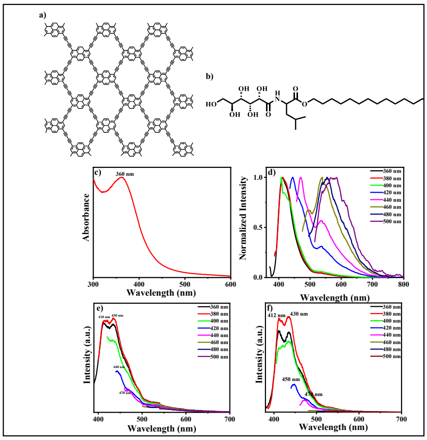

Figure 1. Structure of PDYQDs (a) and OG-leucine (b), emission spectra of PDYQDs in ethanol (c), toluene (d) and (e) recorded at different excitation wavelengths.Text not visible inc,e,e and f

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APPLICATION OF POLYMER-INDUCED AGGREGATION OF RHODAMINE 6G FOR SENSING SULFIDE IONS IN WATER

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Overexposure to sulfide ions is proven to be harmful to human beings [1] as well as to aquatic organisms [2]. In this work, we have designed a highly sensitive sulfide ion sensor in aqueous medium based on a competitive binding approach in which we have utilised an anionic polymer (sodium polyphosphate, NaPP), an optical probe (Rhodamine 6G) and a metal ion (copper). Rh6G undergoes self-aggregation on NaPP surface in a concentration dependent manner. At low concentrations of NaPP, the polymer assists in the aggregation of Rh6G and leads to a spectral change in the absorption spectra and quenching of fluorescence in the emission spectra. The aggregation process on the polymer surface could be modulated in the presence of copper ions. Furthermore, a higher affinity of Cu^{2+} ion towards sulfide ion was exploited here to modulate the aggregation behaviour of Rh6G for ratiometric sensing of sulfide ions in the aqueous medium. The present sensing platform exhibits an extremely low detection limit (45 nM) using a spectrophotometer. This method can also be used to detect sulfide ions by fluorimetric method with an equally low detection limit (67 nM). The present sensor also provides a wide linearity range (0-30 mM). The detection limit of the current sensor is significantly lower than the permissible limit for drinking water set by WHO (15 µM) [3]. This dual-mode sensing approach for important analytes in aqueous media will be highly beneficial for the sensitive detection of sulfide ions in real water samples.

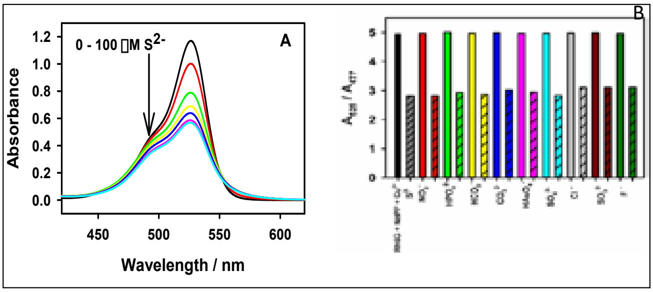

Figure 1. (A) Absorption spectra of Rh6G-NaPP-Cu system in presence of sulphide ions and (B) Selectivity of Rh6G-NaPP-Cu system towards S2- in the presence of different anions

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DECIPHERING THE SYNERGISTIC INFLUENCE OF CONJUGATED RHODANINE ACCEPTORS IN D-D'-A FRAMEWORKS FOR PHOTOVOLTAIC APPLICATIONS

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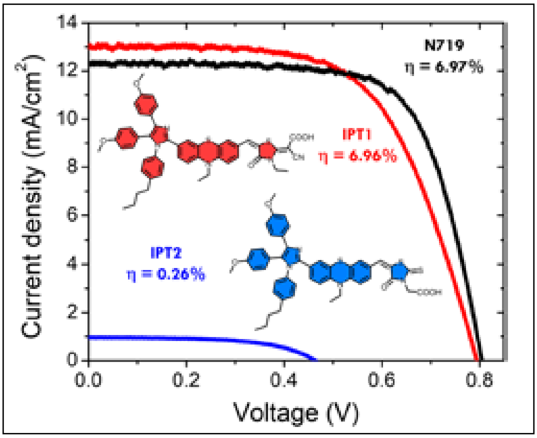

Figure 1. Photocurrent–voltage (J–V) curves of DSSCs based IPT1, IPT2 and N719 dyes (Inset: Structure of IPT dyes with their respective PCE).

The development of photosensitizers with extended π-conjugation, intramolecular charge transfer (ICT) properties, superior light harvesting efficiency and a high molar extinction coefficient in visible region is crucial for achieving high power conversion efficiency (PCE) in dye-sensitised solar cells (DSSCs). In this study, a series of novel dyes featuring imidazole tethered phenothiazine unit as donor and various rhodanine derivatives as an acceptor within a D-D'-A framework have been designed and synthesized. The dyes have been comprehensively characterized using pivotal techniques and contented results were obtained. The objective of the work is to delineate the impact of conjugated rhodanine acceptors on the photophysical and photovoltaic characteristics. Among the investigated dyes, IPT1 exhibited an higher power conversion efficiency (PCE) of 6.96% (J_{SC} = 13.08 mA cm^2 , V_{OC} = 0.793 V, and FF = 0.62) under standard one sun illumination (AM 1.5G, 100 mW cm^{-2}). The PCE is on par with that of the champion N719 dye (h=6.97%). This work demonstrates the exceptional potential of conjugated rhodanine acceptor in D−D′−A-type dye for DSSC applications.

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BIO-INSPIRED METAL-ORGANIC FRAMEWORK (MOF) DERIVED MATERIALS FOR ELECTROCHEMICAL APPLICATION

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In solid state materials chemistry, Bio inspired-materials are extremely important due to their varied topologies, properties, and applications, which include drug delivery, magnetism, sorption, gas separation, enzyme storage and catalysis. These materials are also strengthened by H-bonding and conventional coordination bonding, and they display appealing structural and topological diversities with composite features of individual components. The solvent is a crucial factor that can: a) dictate the structure of complexes and act as a structure directing agent; b) balance the molecules charge upon self-decomposition; and c) give the framework additional stability through H-bonding.[1,2] Herein we represent the Co-BTC-Adenine based Bio-inspired metal organic framework (MOF), featuring a 3D network structure. Co-BTC-Adenine was synthesized by solvothermal reaction condition. The selenylation of Co-BTC-Adenine was carried out at various temperatures ranging from 400°C to 700°C."Among different high temperature annealed product Co-BTC-Adenine@Se_600 shows superior electrocatalytic performance and exhibits a lower overpotential of 180 mV to reach 10 mA cm^{-2} current density in 5M KOH Solution.

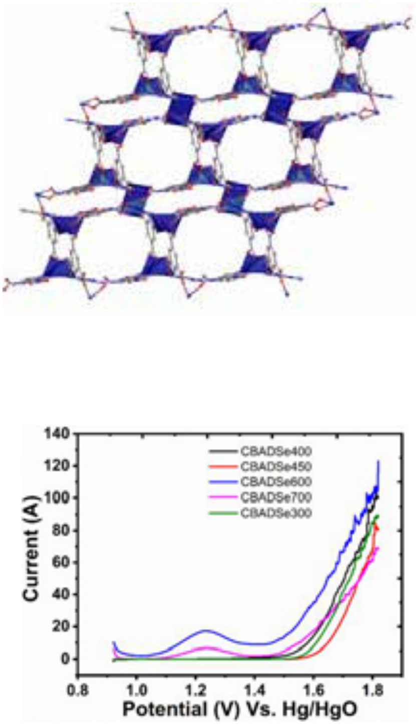

Figure 1. A polyhedral view of a 3D network of Co-BTC-adenine based porous materials. Electrochemical comparison of Co-BTC-Adenine@Se_T in 5M KOH.

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PC - 15

GOLD NANOTRIANGLE TETHERED MONOSTABLE [2]ROTAXANE FOR SELECTIVE FLUORIDE ANION DETECTION

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Compared to the solution phase sensors for cation and anion recognition[1], the field of surface tethered sensors remain less explored[2], which could potentially lead to commercially viable sensing devices. Herein, we report a selectivefluoride ion sensor based on gold nanotriangles (AuNTs) capped with novel pyrene appended monostable [2] rotaxane. The experimental results are summarized in Figure 1. The [2]rotaxane undergoes fluoride ion assisted neutralization causing shuttling of the DB24C8 macrocycle along the axle, which can be detected by a sharp fluorescence quenching of the pyrene monomer and excimer peak, due to the photoinduced electron transfer from the resultant secondary amine. At the same time, the characteristic surface plasmon resonance (SPR) peak of the AuNTs reduce in intensity with concomitant broadening in the long wavelength range upon addition of fluoride ion, indicating possible aggregation owing to charge neutralization. While the bimodal colorimetric and fluorometric sensing is achieved for analyte concentration at submicromolar level, increasing concentration to the millimolar level resulted in visual identification of the aggregate after F^- addition. This current protocol is useful for both organic and inorganic fluoride sensing.

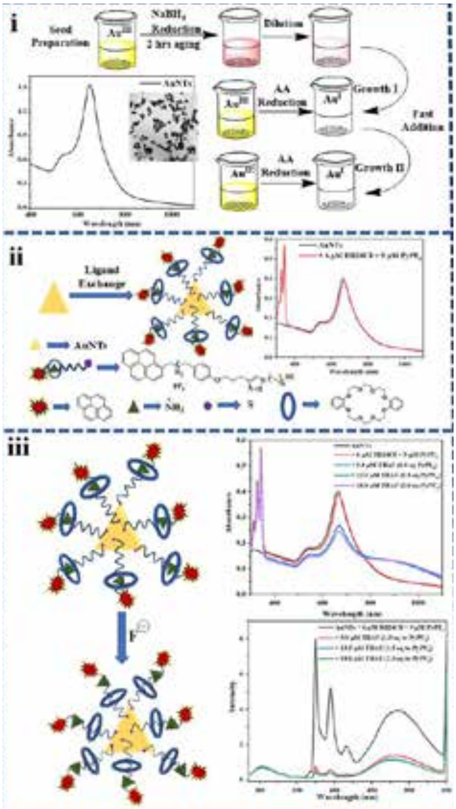

Figure 1. (i) Schematic representation of synthesis of AuNTs by seed mediated method. UV-Vis. spectra and TEM image of AuNTs (ii) Excess CTAC removal and ligand exchange by [2]rotaxane. UV-vis (black) spectra ofCTAC free AuNTs, (red) [2]rotaxane on gold nanotriangle surface, (iii) Effect of Fluoride ion addition to the system and the corresponding response in UV-Vis and fluorescence spectroscopy

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PC - 16

EXPLORING THE SPECIFIC ROLE OF IRON CENTER ON THE CATALYTIC ACTIVITY OF HUMAN SERUM TRANSFERRIN: CTAB-INDUCED CONFORMATIONAL CHANGES AND SEQUESTRATION BY MIXED MICELLES

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Understanding the fundamentals of conformational changes in a protein and their associated biological activities is an indispensable research topic [1]. Herein, we have investigated the conformational changes of an iron-binding protein, monoferric human serum transferrin (Fe-hTF), using several spectroscopic approaches. We could reversibly tune the CTAB-induced conformation of the protein, exploiting the concept of mixed micelles, formed by three sequestrating agents: CHAPS, sodium cholate (NaC) and sodium deoxycholate (NaDC) [2].The formation of mixed micelles between CTAB and these reagents (CHAPS/NaC/NaDC), results in the sequestration of CTAB molecules from the protein environment. However, the guanidinium hydrochloride-induced denatured Fe-hTF did not acquire its native-like structure using these sequestrating agents, which substantiates the exclusive role of mixed micelles in the present study. Apart from this, we found that the conformation of transferrin (adopted in the presence of CTAB) displays pronounced esterase-like activity toward *para*-nitrophenylacetate (PNPA) substrate as compared to native transferrin. We also outlined the impact of the iron center and amino acids surrounding the iron center for the effective catalytic activity in the CTAB medium. We estimated ~3 times higher specific catalytic efficiency for the iron-depleted Apo-hTF compared to the fully iron-saturated Fe_2-hTF in the presence of CTAB.[2]

Figure 1.Pictorial representation of conformational dynamics of human serum transferrin (hTF) induced by CTAB and subsequent sequestration by CHAPS/Bile salts mixed micelles.

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PC - 17

EFFECT OF BIMETALLIC NANOCOMPOSITE SYSTEM (Au@Ag) ON THE ENZYMATIC ACTIVITY MODULATION OF α-CHYMOTRYPSIN

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In the recent years, nanotechnology has emerged as a fascinating branch of science dealing with the study of nano-scale sized systems.Among different nano-architectures, core shell type structures have gained attention because of their improved physical and chemical properties over their singlecomponent counterparts. However, the interaction of core shell type nanocomposite with biological system is still inadequately explored.Thepresent work is undertaken with an objective to find the effect of bimetallic nanocomposites (NCs) systemAu@ Ag on the enzyme activity modulation of a model enzyme, α-Chymotrypsin. For this purpose, Au@ Ag synthesis is done by using GSH as the surface ligand[1]. The interaction of the nanocomposite system with α-Chymotrypsin has been investigated by employing various microscopic andspectroscopic techniques like Fluorescence correlation spectroscopy (FCS), UV-Visible spectroscopy, circular dichroism spectroscopy measurements etc. at both ensemble average and single molecule level[2]. The outcome of this study has demonstrated that Au@Ag NCscan act as an effective nanoscale enzyme activity modulator for various biological applications.Details of these investigations will be presented.

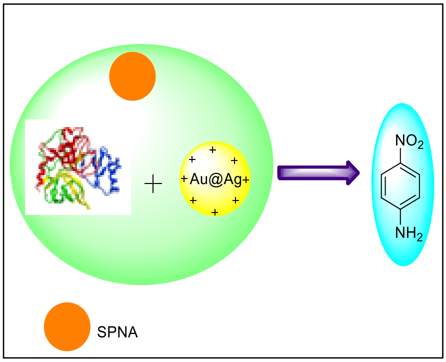

Figure 1. Enzymatic hydrolytic product of SPNA.

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THEORETICAL EXPLORATION OF TWO-DIMENSIONAL MATERIALS FOR OPTICAL, THERMAL AND ELECTRICAL PROPERTIES

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Two-dimensional materials have emerged as the new hotspot for current research interests in material sciences. Since the revelation of graphene in 2004 [1], the scientific community has delved into two-dimensional materials research in the hunt of better and more efficient sensors, photochemical devices, optoelectronic devices and thermoelectric devices. Janus Materials [2] are a kind of 2D material that has been exploited more over its symmetric counterparts because of their out of plane symmetrical characteristics and hinting towards intra piezoelectric effects as well. The current work ongoing on the Janus monolayer TiSeS has been carried out using Density Functional Theory as implemented in Quantum ESPRESSO 7 with GGA-PBE XC functional. GGA-PBE was used as per the suggestion of literature and has been proved to be an excellent functional for carrying out several janus monolayers. The structural optimization of the monolayer yielded the lattice constant to be 3.47 Å corresponding with the literature. The band structure was calculated further to understand the electronic property of the monolayer and it was found to be a semiconductor with a little bandgap. Upon further calculations, the optical properties of monolayer were calculated and the real and imaginary part of the dielectric constant was produced. These 2-D materials are the present pinnacle of innovation and will just thrive higher over time. The theoretical exploration of these materials and the computational simulations are a necessary and crucial step to bring in some extra time and cost cuttings.

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PC - 19

PHOTOPHYSICAL CHARACTERISTICS OF 3-(2,4-DICHLORO-PHENYL)-1-(3-METHOXY-PHENYL)-PROPENONE: EXPERIMENTAL AND COMPUTATIONAL APPROACH

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A Chalcone is one of the open chain flavonoids which exists in large quantity in plants. Chalcone derivatives have profound applications, they are being used in anti-fungal [1], anti-cancer [2-3],anti-bacterial [4-5] activities. Because of such widespread applications of chalcone derivatives, we have conducted extensive spectroscopic investigations on the 3-(2,4-Dichloro-phenyl)-1-(3-methoxy-phenyl)-propenone(3D3MP)molecule.FT-IR and FT-Raman spectra acquiredthrough experimental and theoretical method were analyzed and compared. The DFT method with B3LYP/6-311++G (d, p) basis set is employed to conduct theoretical computations. The theoretically computed wave numbers are subjected to comparison with experimental data. The entire assignment is accomplished with PED (potential energy distribution) analysis of the individual vibration modes. The charge transfer is studied with help of energy gap obtained by energy difference between HOMO and LUMO. With the help of molecular electrostatic potential (MEP) map the reactive sites present in the molecule have been studied.The natural bond orbital (NBO) analysis was performed for the present molecule to obtain the stabilization energy and to study the inter molecular interactions.In addition, the nonlinear optical analysis, Fukui function, localized orbital locator (LOL)electron localization function (ELF) studies have been conducted on 3D3MP chalcone derivative. Molecular docking studies have been conducted against α-amylase, α-Glucosidase and α-Glucosidase receptors.

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SURFACE FUNCTIONALIZED GOLD NANORODS FOR TARGETED PHOTOTHERMAL THERAPY

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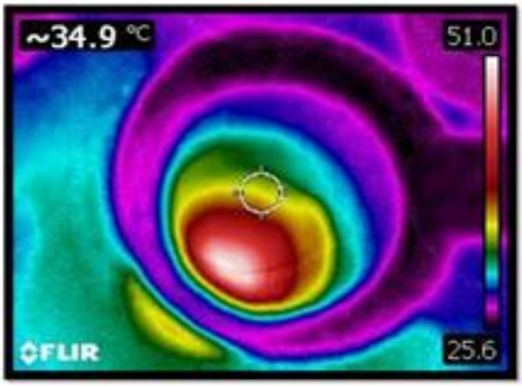

Figure 1. Thermal image of NIR irradiated nanogold.

Cancer is the second leading cause of *death* globally. Despite the huge progress in the field of cancer drugs and therapies, the treatment outcome is still lacking for most cancer patients. In this regard, nanotechnology has revolutionized cancer therapies. Among the different cancer treatment options, lasers have emerged as a promising method for inducing photothermal damage to tumors. Near-infrared (NIR) photothermal therapy (PTT) has gained popularity and has quickly developed in recent years due to minimally invasive patient treatments. NIR irradiation used in photothermal therapy has a greater penetration depth, minimal phototoxicity, and reduced light scattering. Among the available NIR light–responsive nanomaterials, nanogold has become an attractive option owing to its excellent optical properties, ease of synthesis, and outstanding photothermal conversion efficiency. Peptide-conjugated nanogold has been synthesized for photothermal therapy of breast cancer. The nanoparticles have been characterized by FTIR and UV-visible spectroscopy. The nanoparticles have been determined using TEM. The photothermal response of nanoparticles has been tested using laser studies. The cytotoxicity of the nanoparticles was evaluated using MTT assay. The high-performing functionalized nanogold exhibits great potential in tumor targeting and photothermal therapy.

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GAS-PHASE PHOTOLYSIS AND OH REACTION KINETICS OF VINYL METHACRYLATE

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Methacrylates are α, β-unsaturated esters that are widely used in the polymer plastics and resins production. The fate of methacrylates is however poorly understood and scarcely taken into account in atmospheric chemistry modeling. In this work, a combined investigation of the photolysis and temperature dependent OH radical reaction kinetics of vinyl methacrylate (VMC) is presented. The objective was to evaluate the importance of the photolysis process relative to OH oxidation in the atmospheric degradation of VMC. A photolysis lifetime of about 1.1 hours was estimated. The OH reaction rate coefficient follows the Arrhenius trend (268−363 K) and could be modeled through the following expression:

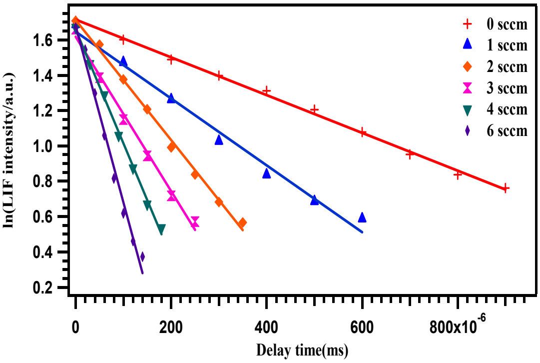

Figure 1.The temporal decay profile of the LIF signal intensity for VMC + OH reaction obtained at 298 K for various concentrations of VMC. Solid lines indicate linear fit.

$$k_{VMC}^{268-363K} = (1.46 \pm 0.6) \times 10^{-12} exp^{[(929.6 \pm 125)/T]} \text{ in cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}.$$

An atmospheric lifetime of 7.2 hours regarding the OH + VMC reaction was evaluated, indicating that photo-dissociation is by far the major degradation channel. The present work underlines the need for further studies on the atmospheric fate of methacrylates.

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PC - 22

FLUORESCENT BASED DETECTION OF ANTIINFLAMMATORY DRUGS USING CAPPED CADMIUM SULFIDE QUANTUM DOTS

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Quantum dots (QDs) are semiconductor particles that have all three dimensions confined to the nanometre scale. They have the capacity to glow or fluoresce brightly when excited by a light source such as a laser. As a result of quantum confinement, they have unique optical and electronic properties such as broad excitation spectra, narrow symmetric, and tunable emission spectra [1, 2]. The synthesis and study of inorganic QDs have become a major interdisciplinary research area in recent years due to their numerous applications in various areas.Semiconductor nanocrystals such asCdSe, CdTe, CdS, and ZnSe, exhibit a vast range of applications, such as light-emitting devices, non-linear optical devices, solar cells, and as fluorescent bio-labels. However, QDs are still facing some unsolved problems such as ultra-sensitivity of their fluorescence to the surface states, cytotoxicity of heavy metal ions used in the process of synthesis which are released upon photo-oxidation, and chemical and colloidal instabilities in harsh chemical environments. Realizing the importance of it, capped and coated QDs attract much attention and core/shell QDs emerged.

Pharmaceutical drugs are biologically active, long-lasting substances that are recognized as emerging contaminants and aninvariant threat to the environment. Every year, tons and tons of drugs are produced and consumed, making them susceptible to leakage into the aquatic ecosystem through wastewaterdischarge from the municipal, healthcare, and pharmaceutical industries, livestock treatments, improper drug removal, and aquaculture practices [1]. Our work explores the utilization of fluorescence techniques and highlights the interaction between the analyte and the quantum dots. Systematic study on the synthesis, characterization, photophysics and photochemistry of capped CdS quantum dots [2] are carried out and subjected for the anlaysis of antiinflammatory drugs (Ketorolac and aspirin). Capped CdS QDs exhibit pronouncing emission properties and the sensing mechanism with the analytes was studied. Effect of various parameters on the recovery of drugs such as amount of capped CdS QDs, pH and stability of the QDs was investigated and validated for screening of drugs in realsamples.

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PC - 23

MOLECULAR-LEVEL CHARACTERISATION OF THE CHALCOGEN BOND INTERACTION: A CASE STUDY OF THIOPHENE WITH DIMETHYLACETAMIDE

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Chalcogen bond (ChB) is the attractive non-covalent interaction between the group 16 elements (O, S, Se) with nucleophiles [1,2]. Recent studies have revealed that chalcogen bonding interactions play diverse roles in biological systems, supramolecular chemistry, and crystal structures. ChB interaction influences the stabilization of protein structure and its interaction with ligands [3]. Crystallographic structures of proteins complexes with thiophene, thiazole, and thiadiazole units as ligandsare obtained manually from the RCSB Protein Data Bank with a resolution of less than 2 Å. A range of 2.8-4.5 Å for the S---O distance and 130˚-180˚ for the δ C-S---O has been considered in searching for C-S---O interaction between protein backbone and ligand. More than 80 PDB IDs are manually selected where the possibility of the formation of ChB is expected. Hence, adetailed analysis of intermolecular S---O interactions has been carried out, starting from the PDB analysis to electronic structure calculations and, finally, experiments on model systems under cold conditions. This study aims to understand the nature of interaction present in the sulfur-containing molecules withdimethylacetamide (DMAc). Herein, matrix isolation infrared spectroscopyand electronic structure calculations have been performed to identify the stable complex of thiophene (THP) and DMAcand to mimic the protein-ligand interactions as obtained from PDB analysis.Experimentally, a red shift of9 cm^{-1} has been observed in the C-O stretching mode (v_{CO}) upon complexation (Figure1). The simulated frequency of the v_{CO} mode of the complex is red-shifted by 11 cm^{-1} compared to the monomer.

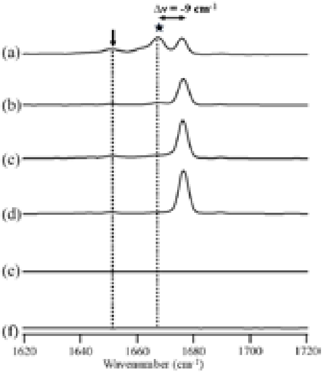

Figure 1The IR spectra recorded in the N2 matrix at 16 K; THP-DMAc mixture after annealing (a), THP-DMAc mixture after deposition (b), DMAc after annealing (c), DMAc after deposition (d), THP after annealing (e), THP after deposition (f). The complex peak is marked with asterisks (*) and the dimer peak is marked with downarrow (↓).

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PC - 24

POLYDOPAMINE-FUNCTIONALIZED IRON OXIDE NANOPARTICLES: SYNTHESIS, CHARACTERIZATION, AND INTERACTION WITH HUMAN SERUM ALBUMIN

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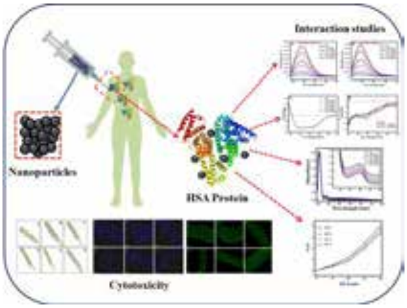

Figure 1.Graphical Abstract: Schematic representation of polydopamine-coated iron oxide nanoparticles and their interaction with HSA.

Iron oxide nanoparticles (IONPs) have been widely investigated for applications in biomedicine, biosensing, hyperthermia, and drug/gene delivery. Due to these diverse applications, functionalizing IONPs with suitable materials remains in significant demand. To achieve optimal functionalization, polydopamine (PDA) was employed for its ability to provide an excellent functionalized surface, absorb near-infrared light, and exhibit adhesive properties to customize the desired functionalized IONPs. The Fe_3O_4@PDA nanoparticles were characterized using techniques such as TEM, FESEM, PXRD, XPS, VSM, and FTIR, confirming the successful attachment of PDA. Human serum albumin (HSA), the major protein in blood plasma, interacts with the delivered nanoparticles. Various spectroscopic techniques and cytotoxicity assessments were used to evaluate the effect of Fe_3O_4@PDA nanoparticles on HSA stability and structure. Circular dichroism (CD) and synchronous fluorescence spectroscopy (SFS) were employed to examine structural alterations. Furthermore, temperature-dependent fluorescence measurements indicated a combination of static and dynamic quenching[1]. A cytotoxicity study on Drosophila melanogaster larvae found no cytotoxic effects, with only a minor genotoxic effect observed at higher concentrations [2].

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PC - 25

BINDING CATIONS AND COUNTER ION'S ROLE IN THE INTERFACIAL WATER NETWORK AROUND DIBENZO-18-CROWN-6 ETHER

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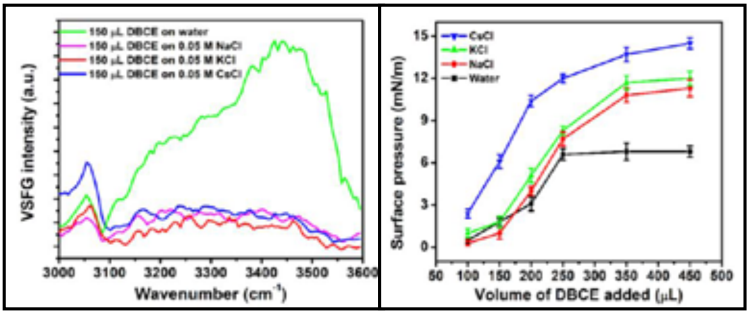

Figure. 1: Changes in the VSFG spectra of water in presence of Benzo 18-crown-6-ether and metal ions; and Surface pressure changes as a result of complexation

Ligand-metal ion complexation requires the transport of metal ions from the aqueous phase to the organic phase. Interfacial water H-bond strength, orientation and dynamics plays a crucial role in this process. The heterogeneity of the air-water interface and its low dielectric constant decides the behavior of interfacial water and is responsible for its enhanced activity [1,2]. Therefore, microscopic picture of interactions happening at the air-water interface is an area worth exploring. In this work, we have studied the changes in the orientation of interfacial water molecules in presence of dibenzo 18-crown-6 ether spread on water surface. Then the corresponding changes are recorded in presence of Na^+, K^+ and Cs^+ ions in the bulk. Further, the effect of counter anion namely Cl^-, SCN^-, SO_4^{2-} on the interfacial water network is also studied. VSFG data revealed that there is an increase in the net polar orientation of the interfacial water molecules. The hydronium ions get encapsulated inside the cavity of the ether and as a result, there is a distribution of positive charge at the air-water interface, leading to polar orientation of interfacial water. In the presence of metal ions in the bulk, metal ions replace the hydronium ions and form an electric double layer (EDL) with the counter anions. The length of EDL is found to be in accordance with the surface propensity of anions, which in turn decides the polar orientation of water molecules. The orientation of interfacial water molecules around the crown complex is found to be weakly dependent on the size of the metal ion. Cs^+ ions are found to have greater influence on the orientation of benzene rings of the ether as suggested by the increasing peak intensity of 3070 cm^{-1} (Fig. 1). Surface pressure measurements (Fig. 1) also suggests that Cs^+ forms an exclusion complex with the ether while Na^+, K^+ form an inclusion complex.

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PROBING THE INTERACTION MECHANISM BETWEEN COPPER NANOCLUSTER AND CALF THYMUS DEOXYRIBONUCLEIC ACID

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The main objective of the present work is to understand the interaction between Copper nanocluster (CuNCs) and Calf thymus Deoxyribonucleic Acid (Ct-DNA). The work is undertaken basically to find out the suitability of CuNCs for biotherapeutic applications[1]. Copper based NCs are chosen as they are biocompatible and cheaper, whereas ct-DNA is chosen due to the fact that it is responsible for gene expression, transmitting genetic information, and driving both the variation and evolution of organisms.For theinvestigation, Tannic acid capped CuNC (TA-CuNCs) and Cysteine capped CuNC (Cys-CuNCs)have been synthesized and characterized by using spectroscopic and microscopic techniques. The interactions between well characterisedCuNCs and ct-DNA have been examined through various spectroscopic methods at both the ensemble average and single-molecule levels. The findings have depicted that the binding mechanisms of two types of CuNCs with ct-DNA are not same. To gain a deeper molecular understanding of the binding interactions, isothermal titration calorimetry (ITC), fluorescence correlation spectroscopy (FCS), and circular dichroism (CD) spectroscopyhave also been employed. Thermodynamic data from fluorescence titration and ITC measurements have indicated that Cys-CuNCs bind to ct-DNA via a one-step process, while TA-CuNCs follow a two-step binding mechanism. Through FCS studies it has been shown that CuNC-CtDNA interaction is also possible at single molecular level. Additionally, CD measurements have been also performedto comment on how the native structure of ct-DNA can be affected in presence of CuNCs. The results of this study underscore the significant role of surface ligands in modulating CuNC-DNA interactions. The findings of this study suggest that CuNCscan act as potential candidates for various biological applications, including gene therapy[2].Details of the investigations related to this work will be presented.

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LIGHT-INDUCED REVERSIBLE INTERCONVERSION OF FCC Ag_{14}NCS TO HEXAGONAL Ag_7NCS: PARTICLE-ASSISTED REVERSIBLE INTERCONVERSION

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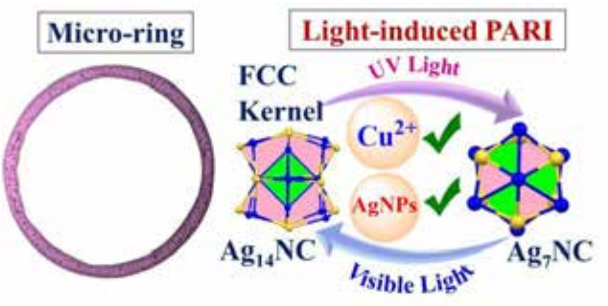

Figure 1.The schematic representation of the work, reflecting the salient features of the present investigation.more specificCaption

Although intercluster conversion in atomically precise metal nanoclusters (MNCs) has gained intense research interest for their associated structural conversion, [1] achieving light-induced reversible structural transformation remains a central challenge and has not been sufficiently addressed. The present investigation showcases a new route for intercluster conversion, a light-induced Particle Assisted Reversible Interconversion (PARI) strategy for the reversible transformation from Face Centered Cubic (FCC) **Ag_{14}NCs** to hexagonal **Ag_7NCs**. Our studies reveal that the lack of plasmonic silver nanoparticles (AgNPs) in the system results in the formation of **Ag_7NCs** with hexagonal centrosymmetric metallic kernels. The molecular self-organization of **Ag_7NCs** through various non-covalent interactions such as C-H•••O, C-H•••H, and C-H•••π leads to the formation of micro-ring morphology, a unique molecular architecture in MNCs. These two structural units of AgNCs show light-induced reversible structural transformation which is also associated with the reversible tuning of their optical properties. This PARI-guided interconversion strategy put forward the most appropriate example of a structure-property relationship in MNCs, enabling efficient reversible structural transformation from FCC structural unit to hexagonal unit and *vice-versa*. Besides, in the absence of Cu^{2+} ions, the obtained **Ag_{14}NCs** undergo UV-light-induced tandem conversion to **Ag_7NCs** and subsequently to **Ag_5NCs**, accompanied by a change in their optical properties. [2]

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TARGETING AMYLOID FIBRILS VIA MACROCYCLIC TEMPLATED SILVER NANOPARTICLES

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Targeting amyloid fibrils either through inhibition of fibril formation or by disintegration of mature fibrils has attracted considerable research interest [1]. A range of supramolecular entities, including cucurbit[7]uril, sulfobutylether β-cyclodextrin (SBE$_7$βCD), and calixarene, have been involved in inhibiting fibril formation. The application of various biomaterials and polymers as coatings on silver nanoparticles has also made significant contributions to the field of fibril inhibition. So, in this aspect, silver nanoparticles decorated with sulfobutyl ether β-cyclodextrin (AgNPSBE$_7$βCD) were synthesized using wet chemical method. It was successfully characterized using UV-vis, FTIR, TEM and zeta potential. Further, *in vitro* synthesis [2] of insulin fibril in absence and presence of AgNPSBE$_7$βCD was monitored using ThT fluorescence assay, which demonstrates a significant increase in fluorescence intensity of ThT by ~250 fold in absence of AgNPSBE$_7$βCD, indicative of fibril formation. While, in presence of AgNPSBE$_7$βCD, no such change in fluorescence intensity was observed as shown in Fig1, which points out the inhibition of fibril formation. This result was further supported with TEM images. Incremental addition of AgNPSBE$_7$βCD to the mature fibril solution, leads to the decrease in the fluorescence intensity of ThT, which suggests the disintegration of amyloid fibril. Highest concentration of blank silver nanoparticle (AgNPs) was added during incubation to study the fluorescence behaviour, but it does not inhibit the formation of fibril. Consequently, silver nanoparticles functionalized with SBE$_7$βCD are poised as exceptionally viable candidates for the disintegration and inhibition of amyloid fibrils.

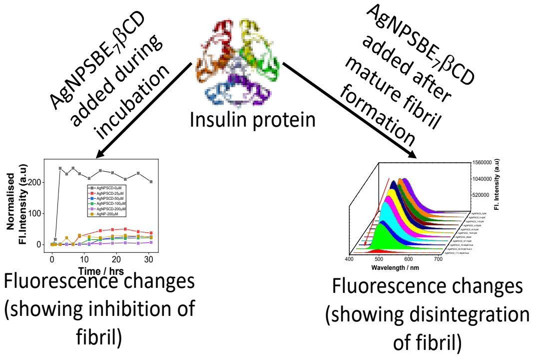

Figure 1. Scheme for the disintegration and inhibition of insulin fibril using AgNPSBE7βCD

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PROTEIN CONFORMATION, DYNAMICS AND FUNCTION: A CORRELATION WITH SHAPEAND SIZE OF MACROMOLECULES

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Macromolecular crowding, characterized by high concentrations of macromolecules within cellular environments, significantly influences protein dynamics and kinetics, affecting processes such as folding, stability, conformational transitions, and interactions. While factors such as pH and temperature have been extensively studied in relation to protein behaviour, the specific influence of macromolecules on protein folding pathways remains relatively under explored. In our study, we investigated the model protein Cellular Retinoic Acid Binding Protein I (CRABP I) in the presence of α-, β-, and γ-cyclodextrins using circular dichroism (CD) and fluorescence spectroscopy at 25°C. Our findings demonstrate that the concentration and size of macromolecules have a pronounced impact on protein conformations, either promoting more compact structures or mitigating the effects of crowding. Additionally, we studied the effect of cyclodextrins on the reversibility of unfolded CRABP I using CD and differential scanning calorimeter (DSC), observing that cyclodextrins maximize the reversibility of the protein's unfolded state. This suggests that cyclodextrins can stabilize or facilitate refolding of the protein when it is prone to unfolding or aggregation [1].

These results underscore the importance of understanding macromolecular crowding in the regulation of protein folding in vivo [2]. Future studies will investigate the structural dynamics of CRABP I using various denaturants and will explore the folding kinetics in the presence of macromolecular crowders of differing shapes and geometries. By elucidating folding mechanisms, intermediate states, distance distributions, and conformational fluctuations, we aim to bridge in vitro experimental insights with the complexities of in vivo protein dynamics [3].

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PROBING AROMATICITY WITH SUPERSONIC JET SPECTROSCOPY

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Aromaticity is a core concept in chemistry that is even introduced in high school textbooks, yet determining the aromaticity order of simple heterocycles like furan, thiophene, and selenophene remains a challenge. In this poster presentation, we highlight the development and first application of a custom-built, mass-selective electronic and vibrational spectroscopy setup at NISER. This state-of-the-art instrument, designed for high-resolution studies of isolated molecules under supersonic jet-cooled conditions, enables precise investigations into the aromaticity of these five-membered heterocycles. To probe aromaticity, we utilized hydrogen bonding as an indicator of electron density within the ring. The strength of π-hydrogen bonds was measured, revealing a correct aromaticity order: selenophene forms the strongest π-hydrogen bond, followed by thiophene and furan. These results suggest that selenophene is the most aromatic, with thiophene and furan ranking lower. This study not only tries to resolve the long-standing debate about the aromaticity order of these molecules but also demonstrates the effectiveness of our new experimental setup. The ability to test both theoretical predictions and experimental data using this advanced technique opens new avenues for studying aromaticity in complex molecular systems.

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DESIGN & FABRICATION OF ECOFRIENDLY R-PE INCORPORATED HYDROGEL STRIPS FOR THE SELECTIVE DETECTION OF Hg^{2+} IN AQUEOUS MEDIA

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Environmentally benignanalytical tool is important in monitoring harmful chemicals in aqueous media, especially drinking water. In this work, we developed a sensitive and selective hydrogel stripfor detecting mercury (Hg^{2+}) ions in water. Hg^{2+} ion is very toxic and found widespread in aquatic environment that gives harmful effects to humans as well as environment.According to WHO guidelines themaximum allowable level of Hg^{2+} ions in drinking water should not exceed 1 µg/L (0.03 µM) [1]. R-phycoerythrin (R-PE) is a red pigment found in *Gracilariaedulis*, was extracted using an efficient ultrasonication method for the first time. The amount of R-PE extracted from this method is found to be 30nm.It is found out that Hg^{2+} ion quenching the fluorescence of R-PE which gives us the way to detect Hg^{2+}ions in complex water systems [2]. The extent of quenching gives a calibration curve in which this estimation of toxicity can be done precisely in water samples. The sensor was highly sensitive and found LOD and LOQ values of 0.1 µM and 0.4 µM respectively. R-PE was incorporatedinto eco-friendly and economical hydrogel, hydroxyethyl methacrylate, and made an analyte strip [3], which greatly enhanced its practical application. The R-PE incorporated hydrogel opened up the possibility of fast, efficient detection of mercury in real water samples originating from different ecosystems. In addition, it shows great fidelity (RMSEP ~ 0.1 µM) and percentage recovery of ~ 99 ±1 %.

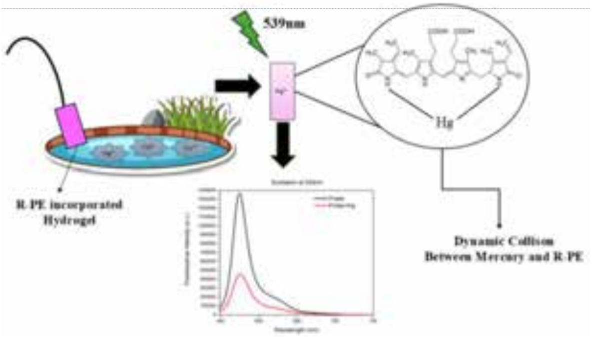

Figure 1. Phycoerythrin-incorporated Hydrogel strip is dipped in water to selectively sense Hg^{2+} ions. The interaction between Hg^{2+} and the hydrogel is highlighted, followed by fluorescence emission spectra, showing quenching upon Hg^{2+} binding

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SPECTROSCOPIC INVESTIGATION ON SOLVATOCHROMISM OF 7-AMINOFLAVONE: AN EXPERIMENTAL AND COMPUTATIONAL APPROACH

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Figure 1. Optimized structure of 7-aminoflavone (7AF).

Flavonoids are a group of polyphenolic compounds, diverse in chemical structure and characteristics, mainly found in fruits, vegetables and cereals. Aminoflavones are a class of compounds that are reported to be highly selective towards breast cancer, and are considered as a new class of anti-cancer agents. The present work is a comprehensive experimental and theoretical study of the spectral and electronic properties of 7-aminoflavone (7AF). The absorption maxima of 7AF appeared in the wavelength range of 282 nm (n-hexane) -353 nm (water) and exhibited a perceptible bathochromic shift with the solvent polarity. Fluorescence spectra of 7AF were also observed in different non-polar and polar solvents which has been observed in the range of 343 - 511 nm. A remarkable bathochromic shift of 9586 cm^{-1} on the fluorescence maximum was observed on changing the solvents from non-polar (n-hexane) to highly polar (water), it signifies the probability of intramolecular charge transfer (ICT) interaction. The ground state and excited state dipole moments of 7AF have been calculated by employing the various solvatochromic shift approaches [1-3]. The dipole moments of the probe molecule calculated using solvatochromic methods were found to be greater in excited state (12.83 Debye) than its ground state (6.88 Debye), which tells us that the ES of 7AF is more polarized. The fluorescence lifetime parameters were obtained at their corresponding excitation and fluorescence maxima are summarized. Furthermore, for better understanding the excited state (ES) behaviour of 7AF, the time-domain measurements were performed in some solvents and it is to be noted that the lifetime τ increase on going from polar aprotic THF (0.92 ns) to polar protic 1-Butanol (3.08 ns) it supports the ICT mechanism. Moreover, the structure of 7AF was optimized with the Gaussian-9 program's package employing the density functional theory (DFT) along with B3LYP functional at 6-311G(d,p) basis set. The optimization energies, geometrical parameters, zero-point corrected energy, and some thermodynamic properties have been estimated to predict the stability of the molecule. Also, some other useful spectroscopic parameters were obtained by the same set of theory based on the optimized structure of 7AF, such as interpretation of electrostatic potential (ESP) map, frontier molecular orbitals (FMOs), dipole moments, NBO, NLO, and electronic transitions etc. Theoretical calculations complement the experimental investigations. Therefore, future research into 7AF as a source of light emitting diodes and fluorescent sensors may have potential applications in the field of optoelectronics.

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ORIENTATION OF HYDROCARBON CHAINS OF TRIBUTYL PHOSPHATE IN BULK AND INTERFACE OF WATER

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Tributyl Phosphate (TBP) is an organo-phosphorus compound which is used as an extractant in the nuclear industry for the extremely important PUREX processfor extraction of uranium and plutonium from ore or reprocessed fuel. Mechanistic details of the process will help understand the technologyfor uranyl solvent extraction in nuclear reprocessing.So far, several groups have studied the mechanism of uranyl solvent extraction theoretically by molecular dynamics simulations or experimentally by surface specific techniques like SFG.

Most of the experimental studies have focussed on the behaviour of P=O bond of the TBP molecules on aqueous interfaces. To corroborate with their results, in this work, we have used VSFG spectroscopy in the C-H stretching region of TBP molecules to investigate air/TBP interface and TBP/aqueous interface.FTIR and Raman spectra were also recorded to compare the bulk medium with the interface. In the VSFG spectrum of pure TBP, recorded at three different polarisation combination, ssp, ppp and sps, five major peaks are seen consistently with different intensities in different polarisation combinations, indicating narrow and well-defined orientation of TBP molecules on air-liquid surface. These peaks have direct correspondence with the Raman and IR peaks with distinct blue shift. This indicates that the interaction between the TBP molecules in air-liquid surface are somewhat weaker than that in the bulk phase.The well-defined positionand intensity along with narrow width of the SFG indicate that the three butyl chains in the interface have similar orientation. Since the phosphate group is highly polar, and the butyl chains are highly non-polar, in air-TBP surface, the phosphate group is expected to reside in the liquid phase, with the butyl chains directed towards the air phase, leading to very narrow conformational and orientational distribution among them.

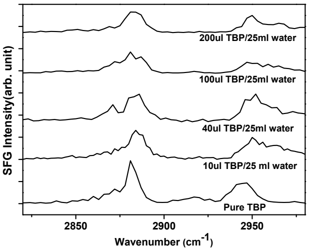

Figure 1. SFG Spectra (ssp)of Interfacial TBP Molecules

Raman spectraof saturated TBP aqueous solution in equilibrium with pure TBP phase gives no signal, suggesting that the aqueous phase has small concentration of TBP. In the Raman spectra of the TBP phase in equilibrium with the aqueous solution, it was observed that the signal of C-H stretching region and the P=O region undergo red shift, indicating the presence of hydrated TBP in the organic layer. It has already been established that the IR signal from the P=O bond of TBP undergoes a red shift in bulk[1] as well as air-water interface[2] due to hydration, The hydration of the P=O bond causes polarisation of the C-H bonds, thus increasing their bond length and eventually red shift in their stretching peaks.

In VSFG spectraof the air-aqueous solution interface,the TBP molecules show uncharacteristic 3cm^{-1} blue shift in the terminal CH_3 group due to TBP-H_2O interaction. This indicates that in the polar environment of the aqueous solvation, the hydrophobic CH chain remains in a more constricted orientation, which leads to the blue shift. Similar blue shift has been predicted in the C-H bond vibration due to interaction with H_2O or other proton acceptors due to improper, blue shifting hydrogen bonding.

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NEW ELECTRON DONOR-ACCEPTOR MOLECULES BASED ON 2-(4H-CHROMEN-4-YLIDENE) MALONONITRILE FOR SENSING AND BIOLOGICAL APPLICATIONS

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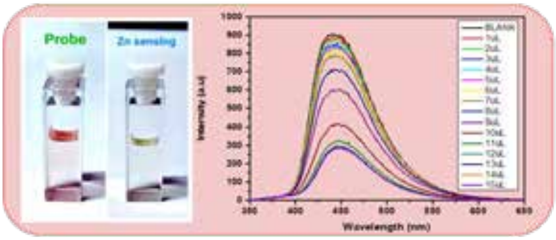

Figure 1. Naked eye and colorimetric detection of zinc ions by AP-1 and AP-2.

Organic molecules with delocalized π-electrons are desirable candidates for developing functional materials for various applications. Organic π-conjugated molecules are inexpensive to synthesize, and their structure-property relationship can be customized to our particular interest, making them ideal candidates in material science. In the past few decades, fluorescent organic π-systems, especially electron donor-acceptor molecules, were successfully employed in optoelectronics, sensors, and bioimaging applications. Two fluorescent sensors, **AP-1** and **AP-2** have been synthesized based on 2-(4H-chromen-4-ylidene) malononitrile electron-acceptor [1] by following well-known chemical reactions such as Vilsmeier-Haack and Knoevenagel condensation [2]. Furthermore, these molecules have been characterized by using FT-IR spectroscopy and mass spectrometry. In addition, photophysical properties were studied systematically using a UV-visible spectrometer and spectrofluorometer. Results show that the two molecules are thermally stable and exhibit strong absorption characteristics in the UV-visible region (300-650nm) and strong fluorescence region (350-650nm) in various solvents. Further, upon screening for detection of different metal ions, these molecules sense selectively for Zinc ions. Among various metal ions, Zinc species are the most prevalent in biological systems [3]. Zinc ion detection has been studied using steady-state and time-resolved spectroscopy. We shall present a complete picture of photophysical properties along with the sensing and biological studies will be presented during the poster session.

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FACET-SPECIFIC PHOTOLUMINESCENCE BLINKING IN PEROVSKITE NANOCRYSTALS

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Photoluminescence (PL) blinking in nanoparticles, usually seen as a limitation for imaging, could be beneficial for next-generation displays if controlled through reversible electron or hole injections from an external source [1,2]. Considerable efforts have aimed at achieving this control by creating a well-defined charged exciton in a nanoparticle using electrochemical charging.Adjusting the rates of photoinduced charging and discharging by changing nanoparticle morphology offers a potentially simple approach to regulating blinking properties, which has not been extensively explored for perovskite nanocrystals (PNCs). This research shows that facet engineering can create PNCs with different morphologies, each displaying unique blinking behaviors. For instance, analysis of single-dot PL intensity trajectories reveals that the fraction of time a PNC remains in the OFF state (r_{OFF}) rises from approximately 0.33 to 0.85 as the number of facets increases from six to twenty-six. This suggests that more facets make PNCs more prone to photocharging due to increased exposure to surrounding materials. This finding is further supported by fluorescence correlation spectroscopy (FCS), which indicates that PNCs with more facets have a higher tendency to bind with nearby molecules that can serve as electron or hole scavengers [3].

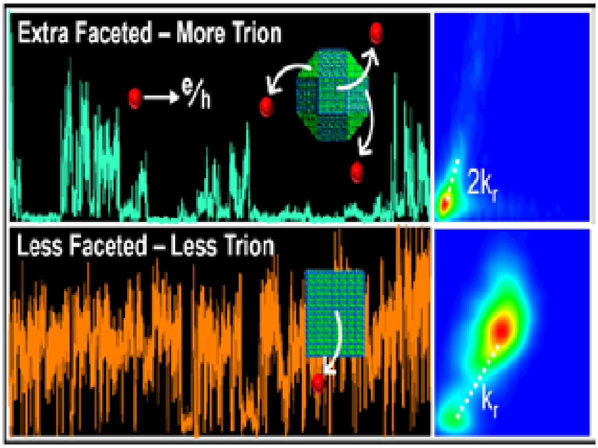

Figure 1.PL intensity trajectories of r-PNC and c-PNC demonstrate a higher density of trion states in the former particle, leading to a prevalence of the OFF-state.

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INTERACTION OF BIOGENIC SILVER NANOPARTICLES WITH BOVINE SERUM ALBUMIN

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Currently, due to their unique applications in a variety of fields, including chemistry, physics, medicine, and biology, nanoscience and technology are attracting significant scientific attention on a global scale. The most noteworthy is the plasmonic nanomaterials, especially the Silver nanoparticles (AgNPs). AgNPs. reveal inimitable physiochemical, optoelectrical, mechanical, and catalytic characteristics due to their high surface area to volume ratio, spatial confinement, and reduced imperfections. The synthesized AgNPs are characterized using techniques like TEM, HRTEM, SAED pattern, XRD analysis, and FTIR spectra. The biogenic AgNPs have an interaction with the most abundantly available bovine serum albumins (BSA). The fluorescent measurement of BSA-AgNP complex depicts the intrinsic fluorescence quenching. The thermodynamic parameters (ΔH, ΔS, and ΔG), binding constant, binding sites were calculated at three different temperatures. The ”–“ve free energy(ΔG) depicts the association of protein-NPs is spontaneous. In the calculation of FRET, the binding distance r lies between 0.5 R_0 and 1.5 R_0 which additionally suggests the energy transferred from BSA to AgNPs. The UV-Vis spectra of protein and protein-AgNPs further implies that there is an association between the proteins and AgNPs in the ground state. FTIR observations also demonstrate the interaction between proteins and AgNPs. The findings of the time-resolved decay profile suggest the static quenching mechanism method. The outcome is in good agreement with the steady-state fluorescence quenching results.

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PHOTOLUMINESCENCE PROPERTIES OF 7-HYDROXYFLAVONE IN AQUEOUS MEDIUM: A FLUORESCENCE ENHANCEMENT STUDY

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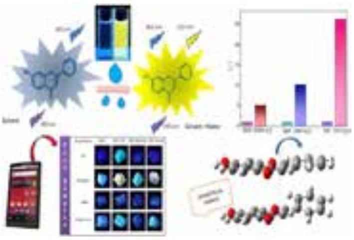

Figure 1. Processes representing 7HF as a water sensing probe

Water is a fundamental and omnipresent molecule, impacting physical, chemical, and biological processes[1].Presence of water impacts a wide range of sectors, from industrial efficiency to environmental conservation, health diagnostics, and scientific discovery.It influences product quality, environmental sustainability, biological health, and safety. Precise monitoring of water content ensures optimal performance in industrial processes, aids in environmental conservation, supports medical diagnostics, and prevents material degradation. Whether in manufacturing, agriculture, or research, accurate water detection is essential for maintaining operational efficiency, ensuring safety, and promoting sustainable practices.Fluorescence techniques are versatile and can be tailored depending on the sensitivity and specificity needed for different environments and systems.Fluorescent sensors showingcolorimetric response may be a good choice for the detection of water, particularly sensing of moisture in organic solvents and raw food materials [1,2]. In view of the potential uses in natural drugs, biosciences, and medicinal practices, Hydroxyflavone (HF) is considered as a group of intriguing organic fluorophores that have made major contributions in the chemical analysis and designing of probes [2].

Photoluminescence properties of 7-hydroxyflavone (7HF) have been explored in different solvents (Dimethyl formamide (DMF), Tetrahydrofuran (THF), Ethanol (EtOH))on varying the water content with steady-state and time resolve techniques.The absorption spectra of 7HF on adding H_2O in different solventsshows the redshift in main absorption band as well as rise in absorbance of longer wavelength region. Fluorescence spectra of 7HF display weak fluorescence in protic and aprotic solvents. Successive addition of H_2O fractions induces fluorescence turn-on response accompanied by the emergence of a new green wavelength band (~527 nm).Quenching plot, Jobs plot and ratiometric plots demonstrated the nature of complexation and fluorescence enhancement of 7HF with H_2O in different solvents.Lower limits of detection of 7HF for H_2O is 0.08% in THF, 0.14% in DMFand 0.389% in EtOH, which is a favorable attribute for practical applications. Time-resolved experiments and theoretical calculations help in understanding the governing parameters involved in the7HF:H_2O complexation, which supports the experimental interpretations to a large extent.The mechanism accounted for the observed fluorescence enhancement of 7HF by H_2O involves hydrogen bonding and anion formation. Additionally, practicalapplication using a mobile phone can make the system quite useful in detecting H_2O in real and commercial samples.Hence, the present study can potentially detect a wide range of water content in organic solvents [2].

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UNDERSTANDING THE ANTIMICROBIAL ACTIVITY OF IONIC LIQUIDS THROUGH ORGANISATION AND DYNAMICS STUDY OF MODEL MEMBRANES

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The antimicrobial activity of the ionic liquid (ILs) is well-known, yet the mechanism of the action remains to be established. Recent research has suggested that the permeabilization of the ILs to bacterial cell membranes is responsible for their ability to kill bacteria. In our study, we examined how the length of the alkyl chain in different ILs affects the structure and behavior of model membranes, in order to better understand the antimicrobial properties of ILs. Here, we have considered four ionic liquids (ILs) i.e. EMIMBr (1-Ethyl-3-methylimidazolium bromide), BMIMBr ((1-Butyl-3-methylimidazolium bromide), HMIMCl (1-Hexyl-3-methylimidazolium chloride) and DMIMCl (1-Decyl-3-methylimidazolium chloride), with different alkyl chain lengths and studied their impact on the organization and dynamics of model membranes. We utilized steady-state and time-resolved fluorescence measurements of two depth dependent probe 1-(4-Trimethylammoniumphenyl)-6-Phenyl-1,3,5-Hexatriene (TMA-DPH, located at the interfacial region of bilayer) and 1,6-diphenyl-1,3,5-hexatriene (DPH, located at the hydrophobic tail region of bilayer), separately. Our results indicate that ILs with longer chain lengths caused greater distortion in the organization and dynamics of model membranes, resulting in higher antimicrobial activity.

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DIMENSION-CONTROL $CsPbBr_3$ PEROVSKITE SYNTHESIS BY TUNING Pb(II) COUNTER ANION AND THEIR APPLICATION IN ORGANIC PHOTOCHEMISTRY

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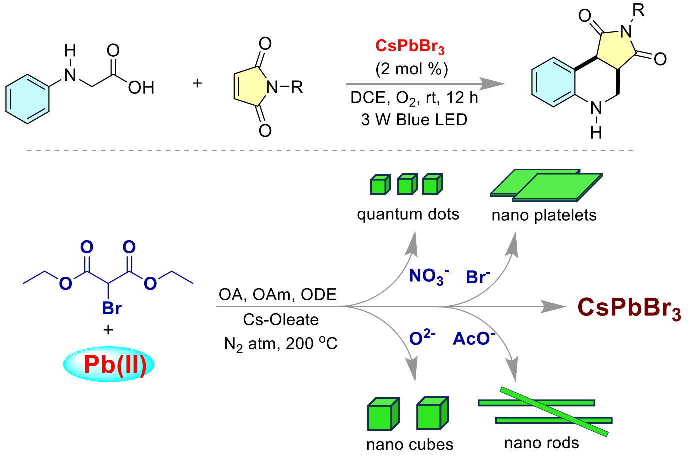

Figure 1. Synthesis of dimension-controlled $CsPbBr_3$ perovskites and their application as a catalyst for photochemical cascade cyclization.

The size modulation of perovskite nanocrystals is a well-established practice in existing literature, achieved through adjustments in reaction temperature, reaction duration, ligand chain lengths, ligand type, halogen source, etc [1,2]. However, our study presents an innovative, inexpensive, and convenient approach to precisely control these nanocrystals' dimensions, encompassing shape, size, and phase, by choosing through the counter anions of Pb(II) during the synthesis via the hot-injection method. For the first time, we employ diethyl 2-bromomalonate as the bromide precursor, and the resultant tunability is attributed to the specific counter anions of the Pb(II) salts. Notably, lead acetate, lead bromide, lead oxide, and lead nitrate yield 1D-nanorods, 2D-nanoplatelets, 3D-nanocubes, and 0D-quantum dots, respectively. Despite the diverse range of sizes and shapes achieved, all $CsPbBr_3$ nanocrystals consistently demonstrate a high photoluminescence quantum yield (PLQY > 90%) with considerable excited state lifetimes ($\tau \sim 6.1 - 15.1$ ns). All the $CsPbBr_3$ NCs exhibit a different extent of photocatalytic performance towards cascade cyclization between *N*-alkyl/aryl-maleimide and *N*-phenyl glycine under visible light irradiation in a non-polar solvent. The yield of the reaction is was directly related to the size and morphologies of the $CsPbBr_3$nanocrystals.

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HIGHLY SENSITIVE AND COLORIMETRIC DETECTION OF MERCURY IONS IN WATER

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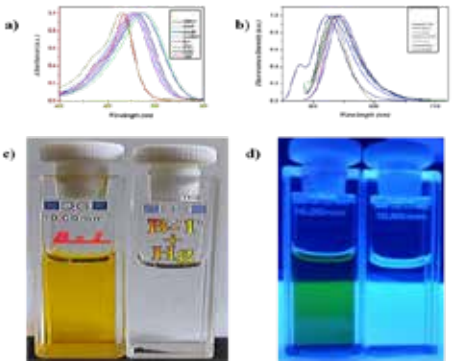

Figure 1. a) & b) Normalized U.V and Fluorescence spectra in low to high polar solvents, respectively, c) & d) pictural representation of naked-eye detection of Hg^{2+} ions in normal sunlight and UV light, respectively.

Mercury is one of the highly toxic, bio-accumulating, and hazardous heavy metals that have adverse effects on various life forms. These adverse effects include enhanced risk for severe brain damage, kidney problems, immune dysfunction and motion disorders in humans. Considering the significance of mercury detection, a new molecular system B-1 has been designed and synthesized from carbamodithioate-based conjugated 1,3 Indanedione molecule-based sensor (B-1) for selective and rapid detection of mercury (Hg^{2+}) in drinking water has been proposed. The **B-1** molecule was synthesized by chemical reactions such as Vilsmeier-Haack and Knoevenagel condensation—further FT-IR, Mass spectrometry and NMR spectroscopy. In addition, photophysical properties were studied systematically using a UV-visible spectrometer and spectrofluorometer and TGA analysis was performed. Results showed that the sensor was thermally stable and exhibited strong absorption characteristics in the UV-visible region (200-550nm) and strong fluorescence in the range of (400-650nm). The sensor responds with a Hg^{2+} coordination interaction between (**B-1**) and Hg^{2+}. The thiol-Hg^{2+} interaction was studied by both UV absorption and fluorescence studies (bulk solutions) of (**B-1**) with increased concentrations of Hg^{2+} (10 nM to 30 μM). The sensor's specificity in the presence of other interfering metals like Pb^{2+}, Cu^{2+}, Na^{2+}, Ag^{2+}, Mg^{2+}, Fe^{2+}, Ca^{2+}, Zn^{2+} Ni^{2+}, Mn^{2+}, Pd^{2+}, Ba^{2+}, Co^{2+}, Sn^{2+} and Cd^{2+} has been determined. The sensor can be used as a highly sensitive, selective, portable, real-time, on-site Hg^{2+} optical probe for drinking water. We shall present photophysical studies as well as sensing applications of the new molecule, **B-1**.

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FLUORESCEIN AS A PHOTOREMOVABLE PROTECTING GROUP: PROBING pH-DEPENDENT PHOTORELEASE AND APPLICATIONS

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Fluorescein dye, with its bright fluorescence, is widely used as a contrasting agent for visualising various biological processes[1].Its various pH-dependent structural forms (e.g., closed, open, monoanionic, and dianionic forms) make the dye more interesting in photophysics and photochemistry [2,3]. To use the interesting properties, we have modified fluorescein moiety as a green light-activated photoremovable protecting group (PRPG), which spatiotemporally releases caged alcohols at a tunable rate by varying the pH of the medium (uncaging quantum yield, ϕ = 0.05-0.005). We have used our PRPG to release bioactive molecules for biological application after developing them as organic nanoparticles to enhance cellular internalisation.

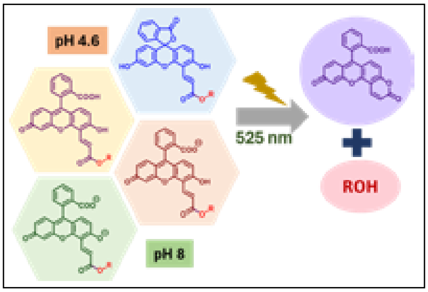

Figure 1. pH-dependent photorelease of caged alcohols from Fluorescein chromophore Cite the figure in relevant sentence of the main text

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SURFACE-IMMOBILIZED SILVER NANOTRIANGLES FUNCTIONING AS PORTABLE SENSING PLATFORM FOR BIMODAL DETECTION OF MERCURY (II) IONS

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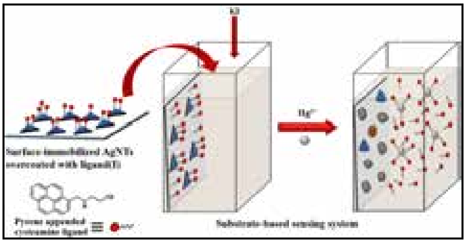

Figure 1. Experimental schematic and the mechanism of Hg^{2+} sensing using surface-immobilized AgNTs exploiting the morphology transition of the nanoparticles due to etching by the halide ions.

We have developed a bimodal colorimetric and fluorometric mercury (II) sensor based on surface-immobilized silver nanotriangles which is simple, robust, portable, and cost effective. This sensory system based on solid substrate exploited the surface plasmon resonance (SPR) response of the silver nanotriangles capped with a pyrene appended cysteamine derivative, the serving as colorimetric and fluorometric marker. Under our optimized reaction conditions, the thiolated ligands were extracted from the nanotriangle surface by Hg^{2+} ions due to higher binding affinity of mercury with the thiol group, which bares the surface of the nanoparticles and make them unprotected to halide etching[1]. The consequent shape transformation[2]of nanotriangles was manifested in the optical response of the surface-immobilized nanoparticles and monitored by UV-visible spectroscopy. The schematic of the sensing mechanism is delineated in Scheme 1. Also, the change of the fluorescence of the ligands, as they were removed from substrate and released in solution by action of Hg^{2+}, provides additional fluorometric response for the same analyte. The solid substrate-based sensing study is also compared with the conventional solution study using same strategy to have more insight into the former like optimization of conditions, sensitivity, selectivity, etc. This study of Hg^{2+} sensing using surface-immobilized silver nanotriangles demonstrates high sensitivity with a limit of detection of 50nM, high selectivity for Hg^{2+}over other toxic heavy metal ions and a wide range (0.1-10µM) detection for the Hg^{2+} ions.

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PHOTOPHYSICAL STUDIES OF PYRENE BASED FLUORESCENT BIOSENSOR INTO LIPOSOMES

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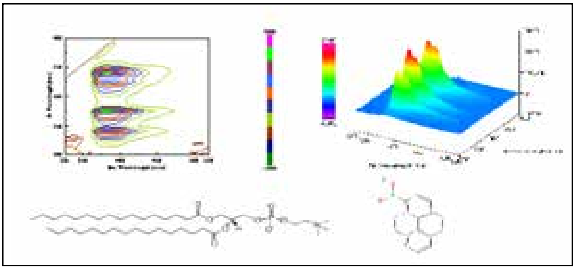

Figure 1. Contour and 3D emission spectra of PBA in DPPC Liposomes

Liposomes are supramolecular lipid assemblies that form an aqueous compartment enclosed by a lipid bilayer membrane are typically in the size of 20 nm to 10 µm in diameter with 4-5 nm thickness. In biosensing applications, liposomes act as an excellent signal transducers of their large surface area and relatively high encapsulation volume. Encapsulation of large amounts of hydrophilic and hydrophobic signalling molecules are important aspect across a wide spectrum of sensing modalities in the bilayer or core, respectively, and amplify the signal. This allows the signal conversions of one-to-one biological binding event to many output signal occurrences. Fluorescence probing is known to be one of the most straightforward, practical, affordable, and less invasive methods for examining the characteristics of lipid bilayers. The specific benefits that fluorescent molecular probes provide high sensitivity, selectivity, rapid response time, non-invasiveness, and minimum perturbance to the microenvironment being probed account for their effectiveness. Conceptually, various types of fluorescence probes have been utilized to investigate various characteristics of lipid bilayer membranes. Development of boronic acid based sensors are great deal of interest, because boronic acids can form tight and reversible complexes with diol compounds such as carbohydrates, etc. According to the different sensory systems, boronic acids are widely employed techniques into five major streams such as i) boronic acid embedded molecular sensors; ii) polymer based sensors iii) boronic acid-functionalized surface; iv) modified nanosensors and v) electrochemical sensors and electrophoresis. Considering the importance of application in the various fields of sensor, we have designed a boronic acid based biosensor. The photophysical characteristics of the boronic acid based sensor into liposomes were studied using spectroscopic techniques.Three dimensional fluorescence technique was employed to study the exact probe location (Figure 1) in the liposomes (DPPC). The pyrene based fluorescent probes were found to be embedded into the liposomes and their binding constant were calculated. The DLS technique was utilized for the conformation of formation and the embedded liposomes with the fluorescent probe.

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FACET ENGINEERING FOR DECELERATED CARRIER COOLINGIN POLYHEDRAL PEROVSKITE NANOCRYSTALS

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After the tremendous success of 6-facet cesium lead bromide ($CsPbBr_3$) perovskite nanocrystals (NCs) in optoelectronic and device applications, recently facet-engineered polyhedral $CsPbBr_3$ NCs have entered the limelight for its unique photophysical characteristics. The rapid cooling of hot carriers (HC) demonstrates an adverse effect on device performance. However, slow HC cooling and extraction of HC can improve the device performance by capturing these carriers much before its thermalization.[1] For example, Cubic 6-Facet $CsPbBr_3$ NCs have a very fast cooling time (0.6-0.7ps) which restricts the HC extraction. Here, facet-engineered polyhedral (12-facet and 26-facet) NCs come into account due to their polaron-mediated slower cooling time as compared to 6-facet NCs which are investigated by femtosecond upconversion technique and TRES analysis. Additionally, very simple HC-extracting molecules like aniline can help in realizing the feasibility of HC extraction much before its cooling.[2]

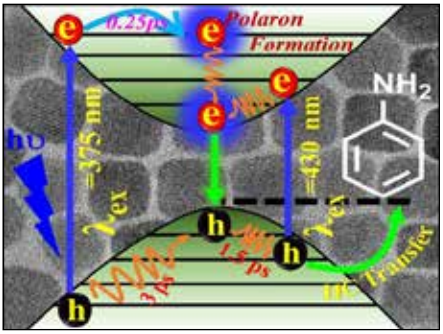

Figure 1. Polaron mediated hot carrier cooling in faceted perovskite nanocrystals.

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HYGROSCOPIC BEHAVIOR OF MIXED INORGANIC $NaNO_3$-$Mg(NO_3)_2$ AEROSOLS

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Atmospheric inorganic mixed salt aerosolsare the topic of a number of fundamental research questions because of their effects in solar insolation, Earth's atmosphere, climate, and health [1]. This study delves into the hygroscopic behaviour, phase changes of 1:1 mixed sodium nitrate-magnesium nitrate $NaNO_3$-$Mg(NO_3)_2$ aerosol particles by micro-Raman spectroscopy. Aerosols were spray-deposited onto Ag substrate placed inside a RH controlled observation cell. The hygroscopic behaviour were studied by drying the particles till 7%RH followed by humidification: equilibrated for 10 mins at each RH interval

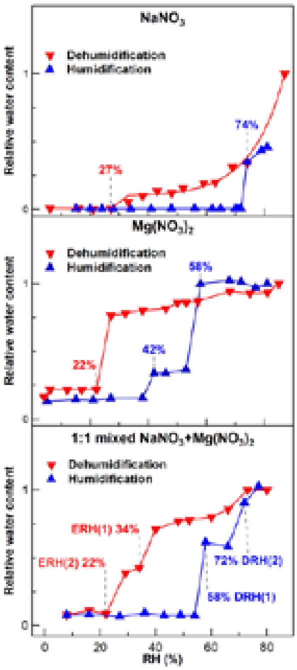

Figure 1. Variation of Relative water content (RWC) Vs RH(%) for $NaNO_3$, $Mg(NO_3)_2$ and NaNO3-$Mg(NO_3)_2$ aerosol particles.

Upon dehumidification, the mixed particles gradually loose water and effloresce in two steps at 34% ERH(1) and 22% ERH(2). Such phase changes in nitrate containing particles can be inferred from the peak shifs in the Raman signatures for $v_{sym.str.}$(N-O). While the $v_{sym.str.}$(N-O)appears at 1049 cm^{-1} for both the nitrate aqueous systems, it blue shifts to 1057 cm^{-1} and 1066 cm^{-1} for solid $Mg(NO_3)_2$ and $NaNO_3$, respectively [2]. ERH(1) is attributed to efflorescence of the $NaNO_3$component of the mixed particles, as confirmed by the appearance of characteristic $v_{sym.str.}$(N-O) at 1066 cm^{-1}. It is interesting to note that the early onset of ERH for $NaNO_3$ in mixed state at 34%, which otherwise appears at 27% in pure system. Upon humidification, the mixed particle deliquesces in two steps with DRH(1) appearing at 58% followed by DRH(2) at 72%. It is inferred from Raman spectral analyses that DRH(1) and DRH(2) correspond to deliquescence of $Mg(NO_3)_2$ and $NaNO_3$ components respectively, in the mixed system. Notably,the behaviour of $Mg(NO_3)_2$ component in the mixed system contrasts that of pure $Mg(NO_3)_2$ aerosols which otherwise take up water in two steps at 42% and 58% RH. These oveservations show the altered hygroscopic behaviour in mixed state of the inorganic salts.The detailed investigations this mixed aerosol system with varying molar ratios will be presented.

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CYSTINE-CORED DIPHENYLALANINE APPENDED PEPTIDE-BASED SELF-ASSEMBLED FLUORESCENT NANOSTRUCTURES DIRECT REDOX RESPONSIVE SITE-SPECIFIC CHEMOTHERAPEUTIC DRUG DELIVERY

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Fabrication of stimuli-responsive superstructure capable of delivering chemotherapeutics directly to the cancer cell by sparing healthy cells is crucial. Herein, we developed redox-responsive hollow spherical assemblies through self-assembly of disulphide-linked cysteine-diphenylalanine (SN). These fluorescent hollow spheres display intrinsic green fluorescence, are proteolytically stable, biocompatible and allow for real-time monitoring of their intracellular entry. The disulphide bond facilitates selective degradation in the presence of high glutathione (GSH) concentrations, prevalent in cancer cells[1,2]. We achieved efficient encapsulation (68.72%) of the anticancer drug doxorubicin (Dox) and demonstrated GSH-dependent, redox-responsive drug release within cancerous cells. SN-Dox exhibited a 20-fold lower effective concentration (2.5 μM) for compromising breast cancer cell viability compared to non-malignant cells (50 μM). The ability of SN-Dox to initiate DNA damage signalling and trigger apoptosis was comparable to that of the unencapsulated drug. Our findings highlight the potential of SN for creating site-specific drug delivery vehicles for sustained therapeutic release.

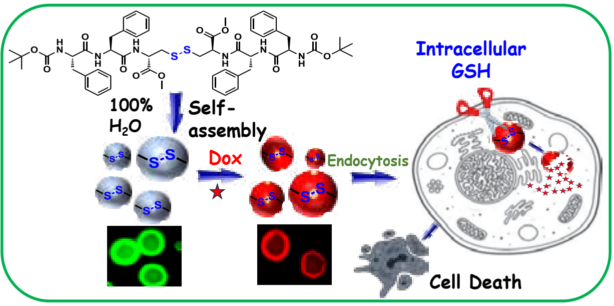

Figure 1. Schematic representation of the formation of SN-based self-assembled hollow spheres, Dox encapsulation, and their application in drug delivery.

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EFFECT OF TRIETHYLAMINE ON THE FLUORESCENCE PROPERTIES OF 3-AMINOBENZOIC ACID

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Amines are critically important and used as corrosion inhibitors, pharmaceutical products, anti-cancer agents, DNA alkylators, cosmetics, toiletries products, colour reprography, and agrochemicals[1]. Triethylamine (TEA) is a derivative of amine, it has several applications viz. raw material in chemical industries, synthesis of various dyes,pesticide production, polymerization inhibitor, organic solvent and curing agents. Meanwhile, it is a highly flammable, toxic and explosive organic compound and can causes great damage to human health such as serious eye irritation and acute skin corrosion and respiratory disorder.Therefore, it is desirable to develop fast and accurate detection technology with high sensitivity and low limit of detection [1,2].In the past, numerousstudies have mentioned the modulation ofphotophysical and photochemical properties of severalorganic molecules(bearing hydroxy and amine groups) with an aliphatic amine (i.e,TEA) [2].

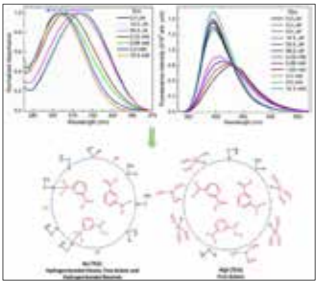

Figure 1. Interaction mechanism of 3ABA with TEA

In the present work, fluorescence propertiesof 3-Aminobenzoic acid (3ABA) were investigated in the presence of TEA. Aminobenzoic acids have a wide range of applications in various research fields such as biology, pharmacy, drug designing, optoelectronics as they possess intramolecular charge transfer/excited state proton transfer nature depending on the molecular geometries [3].The study is followed in aprotic (acetonitrile(ACN)) and protic (methanol (MeOH)) solvents using steady-state and time-resolved techniques. In the presence of TEA, the blue shift in the maximum absorbance while decrease in fluorescence intensity and lifetime of 3ABA was observed due to non-fluorescent H-bonded charge transfer complex/contact ion-pair. Whereas, in MeOH in the presence of TEA blue shift in the absorption and fluorescence spectra of 3ABAwas observed along with the enhancement in fluorescenceintensity but fluorescence lifetime changes merely.These results occur due to H-bonding/anion formation in MeOH because TEA is a strong proton acceptor. The presence of various species which modulate the fluorescence properties of 3ABA significantly depends on the nature of the solvents.Thus, TEA acts as a fluorescence quencher in ACN and enhances the fluorescence intensity in MeOH. Hence, such a molecular system (3ABA-TEA) may have potential application in sensing/recognition of TEA in biological environments.

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OCTUPOLAR CYCLOTRIPHOSPHAZENE-CORED SELF-STANDING COVALENT ORGANIC FRAMEWORK MEMBRANES AS NONLINEAR OPTICAL MATERIALS: IMPACT OF LINKAGE TYPES AND MATERIAL FORMS

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Conjugated and processible self-standing vinylene-linked covalent organic framework membranes (COFMs) are highly demanding for photonics and optoelectronics [1]. In this study, we present the fabrication of the first cyclotriphosphazene (CTP) cored vinylene-linked self-standing COFM, denoted as CTP-PDAN, using a modular temperature-assisted interfacial polymerization approach [2]. To facilitate a direct comparison of physical properties, we also successfully prepared the imine-linked counterpart, CTP- PDA. By leveraging the inherent nonlinear optical (NLO) response of the CTP core, both the COFMs were directly mounted to evaluate NLO parameters using the open-aperture (OA) Z-scan technique with high energy (≅ 5 μJ) ultrashort pulses (≈ 370 fs pulse width at 1030 nm central wavelength) from a near-infrared laser. This direct measurement approach for assessing the NLO response of COFMs is straightforward and advantageous, eliminating significant contributions from solvent and scattering effects, thus enhancing its practicality compared to conventional dispersion mode techniques. The OA Z-scan transmission revealed a reverse saturable absorption (RSA) signature, indicating a higher NLO absorption coefficient (β) of 58.37 cm/GW for CTP-PDAN compared to the imine-linked CTP-PDA COFM (β = 8.5 cm/GW). These findings can be attributed to the relatively planar and uninterrupted efficient conjugation facilitated by the vinylene linkage in CTP-PDAN, as opposed to the quasi-planar imine linkage in the CTP-PDA COFM.

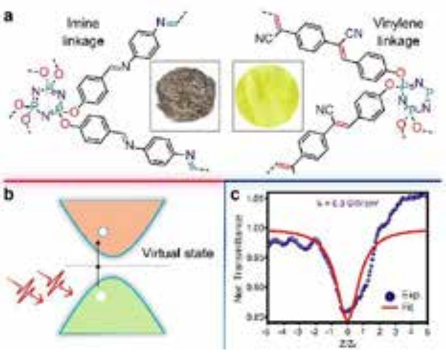

Figure 1. (a) Schematic Representation of COF. (b)Schematic Representation of 2 photon absorption (c) Z-Scan

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CHIRAL SELECTIVE SELF-ASSEMBLY OF NANOCELLULOSE CHIRAL C-DOT FILM SUPERIOR PLATFORM FOR CHIRAL SENSING

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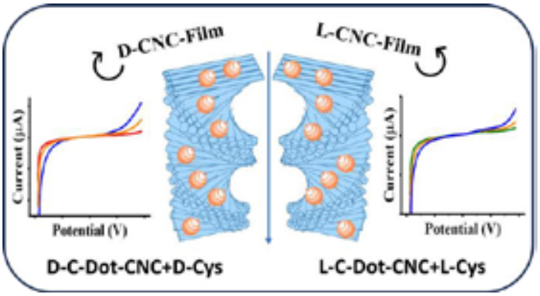

Figure 1. Left and right-handed L/D-C-Dot-CNC composite film for chiral sensing

Chiral detection and sensing using chiral biomaterials is an emerging field of research in advanced bioelectronics [1-3]. Therefore, chiral-controlled biomaterials are essential to enhance the existing technologies in chiral carbon dot (C-Dots) modulated self-assembled emissive cellulose nanocrystals (CNCs) film. Interestingly, the chirality of the CNC film can be tempered between left-handed and right-handed chirality after being doped with chiral L/D-C-Dots in CNCs (C-Dot-CNC film), transferring the chirality from C-Dots to CNCs. The interaction between C-Dots and CNCs and carrier dynamics are investigated using a variety of steady-state and time-resolved PL spectroscopy techniques. The chiral C-Dot-CNC film is formed through evaporation-induced self-assembly of CNCs and this free-standing film is used for electrical studies and sensing applications. The chiral CNC-C-Dots electrodes demonstrate an excellent ability to distinguish between left-handed amino acids and right-handed acids. Moreover, chiral CNC-C-Dots electrodes exhibit approximately two times greater effectiveness in sensing the specific chirality of amino acids compared to the other. These findings on the underlying mechanism of spin selectivity between chiral CNC-C-Dot and chiral ligands hold promise for the development of efficient chiral-sensing devices.

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EFFECT OF VIBRATIONAL STRONG COUPLING ON CIRCULAR DICHROISM: A CASE STUDY ON CAMPHOR ENANTIOMERS

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Polaritons are created due to the strong coupling between photons and excitations within molecules. The photonos could be UV and IR photons, and the excitations could be electronic or vibrational. When IR photons strongly interact with some of the excited normal modes of vibrations of the molecule, it is known as Vibrational Strong Coupling (VSC) that leads hybridized vibro-polaritonic states (VP+ and VP−). The vibro-polaritonic states are separated by the Rabi splitting energy ($\hbar\Omega_R$).VSC provides a novel approach for modifying molecular photophysical and photochemical properties with potential applications in controlling chemical reaction kinetics, chemo and stereoselectivity, ionic conductivity, the rate of vibrational energy transfer, selective crystallization, self-assembly, and solvent polarity. A critical aspect of VSC is understanding how coupling strength and energy dissipation are influenced in systems where vibrational transitions in chiral molecules interact with cavity modes. Our aim is to explore how VSC impacts the behaviour of enantiomers within a Fabry-Perot cavity, focusing on the R- and S- forms of camphor dissolved in carbon tetrachloride solvent. Using the Vibrational Circular Dichroism (VCD) instrument we attempted to explore how it behaves in different circular polarized light. In both the enantiomers of camphor, the C=O and C-H stretching vibrations were on-resonantly coupled with the optical cavity simultaneously. Additionally, we studied the dispersion process by adjusting the cavity path length (detuning).

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UNRAVELING LIPID DROPLET DYNAMICSDURING FERROPTOSIS USING A NOVEL D-A-D FLUORESCENT PROBE

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Lipid droplets (LDs) are crucial cellular organelles involved in lipid metabolism, energy homeostasis, and signal transduction.[1] This work investigates the dynamics and polarity changes of LDs during ferroptosis, a regulated form of cell death marked by iron-dependent lipid peroxidation.[2] Utilizing the terephthalate group based Donor-Acceptor-Donor (D-A-D) fluorescent probe R1 (figure 1, inset), we have conducted real-time visualization of LD behavior in HeLa and A549 cells under various conditions using confocal laser scanning microscopy (CLSM) and Fluorescence Lifetime Imaging Microscopy (FLIM). The results demonstrate that R1 selectively localizes to LDs, providing a robust and sensitive means to monitor LD dynamics. Upon inducing ferroptosis with erastin, a significant decrease in R1 fluorescence intensity as well as lifetime is observed within LDs, indicating increase in polarity, which is a hallmark of ferroptosis. These findings highlight the potential of R1 as a powerful tool for studying LD-related processes, particularly in understanding ferroptosis mechanisms and lipid metabolism disorders. This work establishes the use of R1 for advancing lipidomics research and offers potential applications in disease diagnostics and the development of targeted therapeutic strategies.

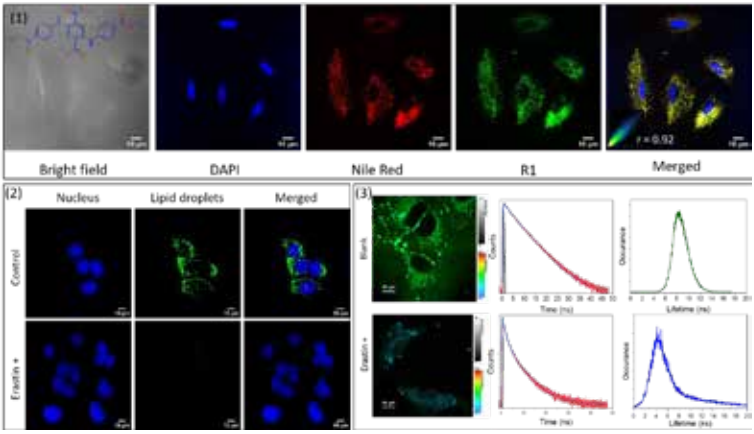

Figure 1. (1) CLSM images of A549 cells treated with Nile Red, and R1.Inset (bright field image): structure of R1. Inset in the merged image of DAPI, Nile red and R1 shows Pearson's correlation plot (r) of Nile Red and R1 fluorescence intensities, indicating co-localization of lipid droplets. (2) CLSM images of A549 cells. Top: Control cells with normal distribution of nuclei (DAPI) and lipid droplets (R1). Bottom: Cells treated with erastin (10 µM, 6 hours) showing altered lipid droplet distribution and nuclei morphology. (3) FLIM images of A549 cells. Top: Control cells showing normal lipid droplet distribution with corresponding fluorescence decay trace and lifetime distribution. Bottom: Erastin-treated cells (10 µM, 6 hours) displaying altered lipid droplet distribution with corresponding fluorescence decay trace and a shifted lifetime distribution, indicating changes in the cellular environment.

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SUSTAINABLE PHOTOCATALYSIS BY EARTH-ABUNDANT OUTER AND INNER TRANSITION METALS

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Use of less-abundant earth outer and inner transition metal as catalysts in synthesis of organic compounds is widespread in chemical industries, nevertheless, is not environmentally sustainable. Hence, photocatalysis by earth-abundant outer and inner transition metals like iron(III)chloride and cerium(III)chloride has been an active area of research for diverse organic transformations[1,2]. Despite these extensive investi-gations, the mechanism of photocatalysis by iron(III) and cerium(III) chloride still remains obscure.

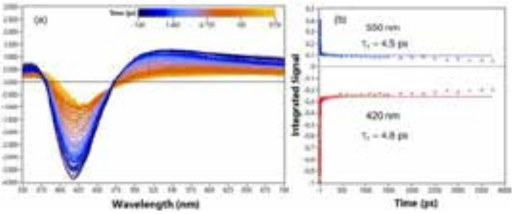

Figure 1. (a) Time-resolved electronic absorption spectra of iron(III) chloride in acetonitrile solution photoexcited with 430 nm pump wavelength. (b) Kinetics at 420 and 550 nm probe wavelengths.

For example, in iron(III)chloride, upon photoexcitation in the LMCT absorption region it was speculated that Fe-Cl bond dissociates to form Cl• radical and reduced iron(II) species. The Cl• radical formed was hypothesized to activate the C-H bonds of both aliphatic and aromatic substrates by H-atom abstraction. But our recent time-resolved absorption spectroscopy study suggests that majority of the LMCT excited state undergoes charge recombination to the ground electronic state while the remaining forms trapped [Fe(II)--Cl•]* species (see Figure 1) is responsible for its photocatalytic activity.[3] Furthermore, our studies unravel that the single electron transfer from toluene to the trapped [Fe(II)--Cl•]* is the rate determining step in the developed photooxygenation approach in contrast to most widely hypothesized H-atom abstraction by chlorine free radical. Additionally, cerium(III)chloride a potent photo-reductant upon UV irradiation has been explored for various organic transformations.[2] Our recent time-resolved absorption spectroscopy study of cerium(III)chloride in acetonitrile and methanol solutions revealed that its ability to photoreduce the halobenzene is subtle to solvents. In this presentation, I shall discuss our more detailed investigation on the photocatalysis mechanism of iron(III) chloride and cerium(III) chloride using time-resolved absorption spectroscopy for various organic transformations.

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SYNTHESIS AND FUNCTIONALIZATION OF EXTENDED π CONJUGATED FLUORESCENT DYES FOR TARGETED ORGANELLE IMAGING

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The study of subcellular organelles is crucial for understanding cellular processes and their implications for health and disease. Effective imaging of organelles, such as the endoplasmic reticulum (ER), lipid droplets (LDs), and mitochondria, enables researchers to elucidate dynamic interactions and metabolic pathways, contributing to our knowledge of phenomena like apoptosis and lipid metabolism. We discuss synthesis of novel extended π-conjugated fluorescent dyes, their photophysical properties and investigate their applications for targeting the organelles. The goal is to develop dye styryl dyes with bright emission and large Stokes shifts, optimizing their performance for cellular imaging and sensing applications. Further, the potential of these dyes for utilization with other imaging modalities will be discussed

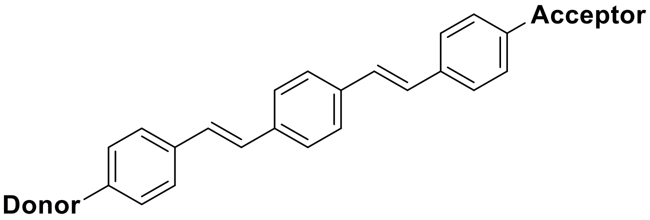

Figure 1. Representative image of the Extended π-Conjugated substrates with distyrylscaffold

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SOLVENT-DRIVEN PHOTOPHYSICS AND COMPUTATIONAL STUDY OF AN AMINOQUINOLINE DERIVATIVE

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This study integrates solvatochromic and computational analyses to elucidate the photophysical and nonlinear optical (NLO) properties of 6-aminoquinoline (6AQ). Fluorescence spectroscopy in various polar and non-polar solvents revealed pronounced solvatochromism in both absorption and emission spectra of 6AQ, with the Stokes shift increasing alongside solvent polarity. This shift indicates a more polarized excited state, potentially involving significant geometric rearrangements and π→π* transitions. Dipole moments in the ground and excited states were quantified using solvatochromic shift methodologies [1].The excited state dipole moment exceeds the ground statedipole moment, indicating enhanced polarization due to ICT and potential alterations in molecular geometry upon excitation.

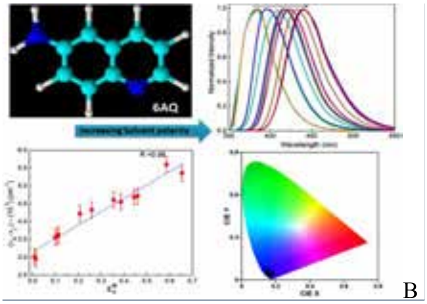

Figure 1.Effect of solvent polarity on the spectral properties of 6AQ.

Catalan scale analysis further elucidates the effects of both non-specific and specific interactions on 6AQ’s spectral properties. Moreover, the compound demonstrates a favorable band-gap energy and CIE chromaticity coordinates in the blue region, nearing the National Television Standard Committee (NTSC) ideal blue coordinate [1,2]. Complementing the experimental data, a DFT/TD-DFT study was performed to explore the molecular properties of 6AQ. TD-DFT simulations, coupled with the PCM model, estimated absorption maxima and emission maxima, with both showing bathochromic shifts as solvent polarity increases. The lowest excited state was identified as a π→π* charge-transfer state, with significant ICT contributing to the stabilization of the molecular system. Additionally, NLO properties, including polarizability, first-order hyperpolarizability, and dipole moment, were computed, indicating that 6AQ is a promising candidate for NLO applications [2]. In conclusion, the synergy between experimental solvatochromic analysis and computational DFT/TD-DFT simulations offers a comprehensive understanding of 6AQ’s photophysical properties. This integrated approach not only corroborates the solvent-dependent behavior of 6AQ but also highlights its potential in optoelectronic applications.

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FLUORESCENT BASED HYDRAZIDE SCHIFF BASE FOR SELECTIVE DETECTION OF ANTIBIOTIC RESIDUES IN FOOD SAMPLES

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Veterinary Antibiotics are a class of medication specifically designed to combat bacterial infections by killing the bacteria and spread within the body of animals [1]. Therefore overuse of these antibiotic will accumulate these drugs in animal-derived products such as milk and eggs, causes risk in human health [2]. Our work particularly focused on synthesizing a new fluorescent hydrazide molecule (ONH) for the detection of antibiotics residues (Tetracycline and Sulfamethoxazole) in food samples. The structure of the synthesized molecules wereconfirmed and characterized by single crystal X- ray diffraction, HR-MS, NMR, IR and UV-Visible spectroscopy. Within the realm of small-molecule based fluorescence sensor systems, particularly utilizing the hydrazide molecule fluorophores, which have garnered substantial attention within the research area due to the p→p*transition which is responsible for the fluorescence nature of the synthesized molecule. This molecule can be attributed to their simple synthesis, facile functionalization, and exceptional photophysical characteristics. Hydrazide derivatives, belonging to the fascinating class of heterocyclic fluorophores, exhibit pronounced absorption and emission properties within the visible region. With wide-range of applications as sensor materials, establishing their significance within the field of fluorescence sensing, our approach involves utilizing luminescence technique and studying the interaction between the analyte (milk and egg samples) and the molecule by fluorescence turn-on/off mechanism. This comprehensive method aims to contribute significantly to the field of antibiotic detection and its potential impact on food safety andpublic health.

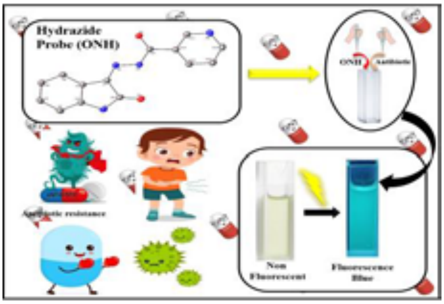

Figure 1. Schematic representation of the detection of antibiotic using Hydrazide fluorescence probe

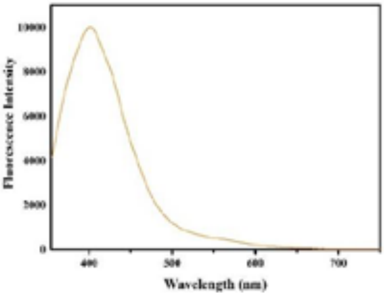

Figure 2. Emission spectrum of the synthesized Hydrazide Probe (ONH)

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SARS CoV-2 FUSION PEPTIDE PROMOTES HEMIFUSION FORMATION IN A CHOLESTEROL-DEPENDENT FASHION

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Membrane fusion is considered the first step in the entry of enveloped viruses into the host cell to cause infection. SARS-CoV-2 fuses at the cell surface by utilizing the fusogenic ability of the spike (S) protein[1]. The S protein undergoes proteolytic cleavage leading to the separation of S1 and S2 protein. The S1 protein binds with the cell surface receptor whereas the S2 protein interacts with the host cell through its N-terminal peptide (fusion peptide) and induces fusion. The importance of N-terminal fusion peptide in viral entry is established for other class I viruses such as influenza and human immunodeficiency virus. In this work, we have evaluated the effect of SARS-CoV-2 fusion peptide in polyethylene glycol (PEG)-mediated fusion of small unilamellar vesicles with varying lipid compositions. Interestingly, the peptide binding to the membrane does not alter the double-layer charge as observed from the measurement of zeta potential. Therefore, the fusion is majorly catalyzed through the interaction between the peptide and the membrane. We have further studied the effect of SARS-CoV-2 fusion peptide on the depth-dependent membrane organization and dynamics utilizing arrays of steady state and time-resolved fluorescence spectroscopic techniques [2]. Our results demonstrate that the fusion peptide promotes fusion by disordering the interfacial region of the membrane, and its disordering ability depends on the lipid composition. Overall, our work provides a better mechanistic understanding of SARS-CoV-2 fusion with the host cell vis-à-vis viral entry.

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SULFATION OF HYALURONIC ACID RECONFIGURES THE MECHANISTIC PATHWAY OF BONE MORPHOGENETIC PROTEIN-2 AGGREGATION

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Bone morphogenetic protein-2 (BMP-2) is a critical growth factor of bone extracellular matrix (ECM), pivotal for osteogenesis. Glycosaminoglycans (GAGs), another vital ECM biomolecules, interact with growth factors, affecting signal transduction. Our study focused on hyaluronic acid (HA), a prevalent GAG, and its sulfated derivative (SHA). We explored their impact on BMP-2's conformation, aggregation, and mechanistic aggregation pathways using diverse optical and rheological methods. In the presence of HA and SHA, the secondary structure of BMP-2 underwent a structured transformation, characterized by a substantial increase in beta-sheet content, and a detrimental alteration, manifesting as a shift towards unstructured content, respectively. Although both HA and SHA induced BMP-2 aggregation, their mechanisms differed. SHA led to rapid amorphous aggregates, while HA promoted amyloid fibrils with a lag phase and sigmoidal kinetics. Aggregate size and shape varied; HA produced larger structures, SHA smaller. Each aggregation type followed distinct pathways influenced by viscosity and excluded volume. Higher viscosity, low diffusivity of protein, and higher excluded volume In the presence of HA promote fibrillation having a size in the micrometer range. Low viscosity, high diffusivity of protein, and lesser excluded volume lead to an amorphous size aggregate in the nanometre range.

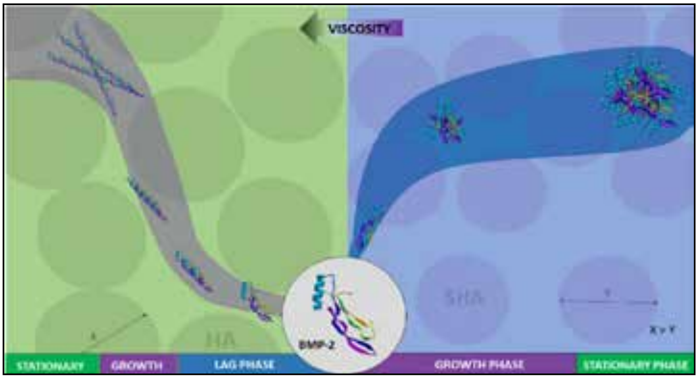

Figure 1. BMP-2 forms amyloid aggregates with HA and amorphous aggregates with SHA, following distinct pathways due to differences in viscosity and excluded volume.

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NAPHTHALIMIDE: A NOVEL ESPT-DRIVEN PHOTOREMOVABLE PROTECTING GROUP FOR CONTROLLED RELEASE OF ALCOHOLS

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Excited state proton transfer (ESPT) is an interesting photophysical phenomenon widely exploited in biological systems, particularly for designing fluorescent probes with reduced background fluorescence [1]. We have utilised this phenomenon in developing a new green light-activated photo removable protecting group (PRPG) based on Napthalimide chromophore, with a phenolic -OH functional group at C-6 position, for the release of caged alcohols with moderate uncaging quantum yield (φ~0.08). This strategic modification of the chromophore shifts its absorption maxima towards the green region as well as incorporates the ESPT phenomenon that results in a large Stoke shift [2,3]. We have also formulated our PRPG as organic nanoparticles for the release of bioactive molecules, which exhibit better cell penetrating ability.

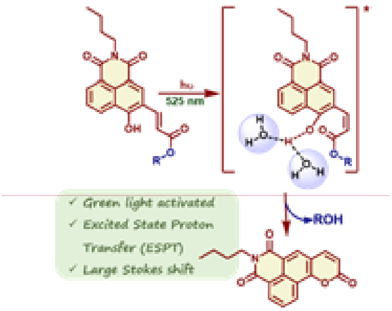

Figure 1. Graphical abstract: BMP-2 forms amyloid aggregates with HA and amorphous aggregates with SHA, following distinct pathways due to differences in viscosity and excluded volume.

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AGGREGATION INDUCED EMISSION ENHANCEMENT BASED FLUORESCENT PROBE FOR THE DETECTION OF HYPOCHLORITE ION

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Fluorescent probes are extensively used for accurate tracing of hypochlorite present in environmental, food and biological samples and have gained considerable interest in the past decade to protect the ecosystem, guarantee food safety and prevent disease [1,2]. A pyrene based Schiff base probe (PT) was developed and expected to display a remarkable emission enhancement upon the interaction with hypochlorite (ClO-). The emission spectrum shows an enhancement and is based on the aggregation induced emission enhancement (AIEE) mechanism. The interaction studies of PT with ClO- are further investigated with various techniques such as UV-absorption, emission spectroscopy, and Fourier transform infrared spectroscopy (FT-IR). PT probe exhibits a notable binding constant, and limit of detection (LOD) values which confirms the sensing ability of the probe developed. Consuming foodstuffs with hypochlorite can lead to food toxicity and life-threatening diseases in humans. Thus, PT is further configured for the detection of hypochlorite residues present in foodstuffs (real sample analysis).

Figure 1. AIEE based fluorescent probe for detection of sodium hypochlorite

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PC - 60

SYNTHESIS, CHARACTERIZATION AND PHOTOPHYSICAL STUDIESON LEAD-FREE INDIUM DOPED SILVER-BISMUTH-BASED DOUBLEHALIDE PEROVSKITENANOCRYSTALS

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In recent years, lead halide perovskite nanocrystals (PNCs) have emerged as the promising materials for optoelectronic applications. However, there are still numerous issues associated with PNCs such as toxicity, low photoluminescence quantum yield (PLQY) and poor chemical stability. These issues have limited the use of these materials for various applications. To avoid these issues, we aim to design a less toxic, highly stable and environment friendly $Cs_2AgBiBr_6$ (which exhibits indirect bandgap nature) double-perovskite nanocrystals (DPNCs) [1]. The In(III)-doped $Cs_2AgBiBr_6$ DPNCs having general formula Cs2AgBixIn1$_{-x}$Br$_6$ (wherex=1,0.75,0.5,0.25) have been synthesized by hot injection method. All the fabricated DP NCs sample have been investigated by using several analytical techniques such as Time-correlated Single Photon Counting (TCSPC), Powder X-Ray Diffraction (PXRD), Transmission Electron Microscopy (TEM), Cryogenic Fluorescence studies, etc. Significant increase in the photoluminescence (PL) intensity and lifetime of the DPNCs have been observed. It has been found that he PL intensity is increased by~70 times and lifetime of DPNCs increase with increasing indium concentration. Interestingly, at low temperature, the dopped DPNCs exhibit dual emission. Cyclic Voltammetry studies show a blue shift in the absorption spectra of DPNCs with increase in indium contents indicating the increase in the bandgap. Additionally, the dual-emission photoluminescence spectra of DPNCs at cryogenic condition has been discussed [2]. In summary,this work underscores the significant influence of indium doping on the structural and optical characteristics of $Cs_2AgBiBr_6$ nanocrystals, presenting them as promising candidates for optoelectronic applications.

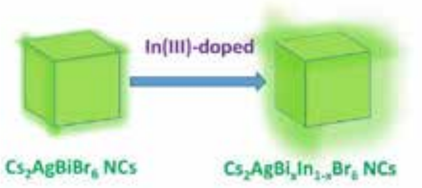

Figure 1. Photoluminescence of Cs2AgBiBr6 NCs after In(III) doping

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ARTIFICIAL LIGHT HARVESTING SYSTEM BASED ON CASCADE FRET IN DNA TEMPLATED MULTICHROMOPHORIC SUPRAMOLECULAR ASSEMBLIES

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Artificial photofunctional materials based on Förster Resonance Energy Transfer (FRET) have been utilized in various fields like photovoltaics, photocatalysis, temperature sensors etc [1,2]. This work focuses on the demonstration of cascade FRET utilizing three chromophoric antennas (DAPI, StyIn, EtBr) and a biological scaffold (dsDNA) as the template. DAPI acts as terminal donor from which energy is transferred to EtBr via StyIn intermediate.

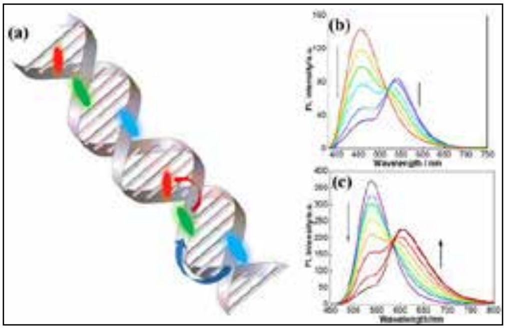

Figure 1. (a) Schematics for cascade FRET, (b) emission change in DAPI-StyIn system, and (c) emission change in StyIn-EtBr system

In presence of dsDNA, addition of StyIn to DAPI solution, the emission intensity of DAPI (~455 nm) gradually decreased, while the emission around the characteristic peak of StyIn (~537 nm) increased. Further, addition of EtBr to StyIn solution results in decrease of StyIn peak (~537 nm) along with increase in the peak intensity of EtBr (~610 nm). Also, the energy transfer for both the steps were monitored by excited state lifetime measurements. The excited state lifetime of donor molecules was found to decrease for both the steps which confirms additional non-radiative channel in the form of FRET. The overlap integral (J(λ)) of absorption and emission spectra of StyIn with DAPI emission and EtBr absorption spectra shows large values. As a result, the fabricated DNA templated multichromophoric supramolecular assembly have found to exhibit high FRET efficiencies as well as high antenna effect (AE) for both the steps.

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ELUCIDATING THE ROLE OF SOLVENT ON THERMALLY-ACTIVATED DELAYED FLUORESCENCE

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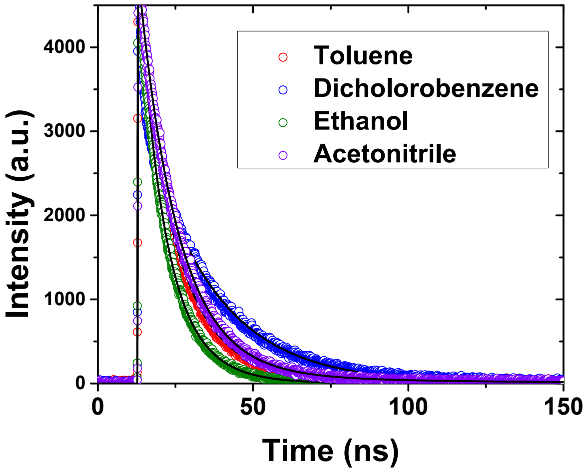

Figure 1.Time-resolved photoluminescence decay of TADF molecule in a range of solvents (Toluene, Dichlorobenzene, Ethanol, Acetonitrile).

Third-generation OLEDs based on thermally activated delayed fluorescence (TADF) has received enormous attention in display technologies.The singlet-triplet energy gap in TADF materials is so small that the weakly emissive triplets could be thermally converted into highly emissive singlets via reverse intersystem crossing (rISC). Solvent polarity and viscosity dependent emission spectra and lifetime suggests that the excited states is polar in nature and associated with structural reorganisation. However the specific role of solvent polarity and viscosity thatdriveTADF emission and associated structural changes are still unclear. We are currently investigatingphotodynamics of TADF emission in a library of solvents with a) different polarity (while keeping viscosity constant) and b) different viscosity (while keeping the polarity constant). Through the steady-state and time-resolved emissionstudies, as shown in Fig.1, we found interesting correlations between emission intensity and itslifetime. This will provide a detailed understanding of the solvent dependency of TADF molecular configurations and aid in designing novel TADF materials with controlled and improved efficiency.

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THE ULTRA-SMALL METAL NANOPARTICLES SUPPORTED ON N-DOPED CARBON FOR PHOTO-CATALYTIC DEGRADATION OF ORGANIC DYES AND NITROPHENOL REDUCTION

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The synthesis of ultra-small metal nanoparticles supported on N-doped Carbon is crucial due to their unique properties and catalytic applications. The ultra-small metal (such as Silver, Gold etc.) nanoparticles were prepared by ultrasonication method. These metals nanoparticles-N-doped carbon demonstrated excellent catalytic activity in the reduction of 4-nitrophenol in aqueous solutions with sodium borohydride ($NaBH_4$), exhibiting rapid kinetics and strong stability. The MNPs–N-doped carbon composite also displayed outstanding photocatalytic degradation of various dyes (RhB, MB, and MR) under UV, visible light, and natural sunlight, with high degradation rates even at high dye concentrations. We anticipate that these MNPs–N-doped carbon composite will be valuable for water purification applications.

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GAS-PHASE NUCLEOPHLIC ABSTRACTION OF HYDROGEN BY OZONE IN SATURATED HETEROCYCLES

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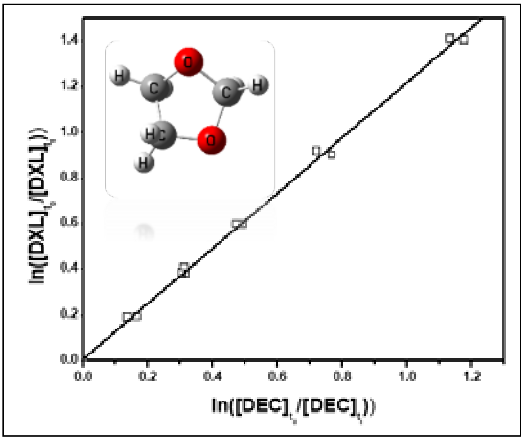

Figure 1: Relative rate plot of the reaction of 1,3-dioxolane with O_3 using trans 1,2-dichlotoethylene as reference compound

Gas-phase oxidation with ozone plays a significant role in the tropospheric degradation of unsaturated VOCs. The chemistry of such reactions is governed by addition of ozone to the double bonds to from primary ozonide which decomposes rapidly into a Criegee intermediate and a primary carbonyl compound. However, the reaction of ozone with saturated heterocycles still remains a scarcely explored arena. Unlike in alkenes, where there is overlap of the highest occupied molecular orbital of alkene and the lowest unoccupied molecular orbital of ozone, such an interaction is energetically less favorable in alkanes [1,2]. A fast 1,3-dipolar addition pathway for ozone reaction with unsaturated compounds leads to their higher reactivity than their saturated analogues. But saturated compounds with electronegative atoms can react with ozone with sufficient reactivity. In this work, we have explored the gas-phase reaction of ozone with series of saturated heterocycles namely 1,3-dioxolane, 2-methyl-1,3-dioxolane, 2,2-dimethyl-1,3-dioxolane. Different molecules are chosen in order to understand the reaction mechanism as well as to understand the factors affecting the reactivity. Unlike unsaturated VOCs, saturated molecules are found to react with ozone via nucleophilic abstraction mechanism. The experimental rate coefficient determined by Gas-Chromatography for 1,3-dioxolane and 2-methyl-1,3-dioxolane is found to be $(2.1 \pm 0.9) \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} and $(5.3 \pm 0.5) \times 10^{-19}$ cm^3 $molecule^{-1}$ s^{-1} respectively. 2,2-dimethyl-1,3-dioxolane did not react with ozone under similar experimental conditions. This reactivity trend unambiguously points out that the reaction of dioxolanes with ozone proceeds through the abstraction of hydrogens from the C-H bonds alpha to both the oxygen atoms in the five membered ring. From the theoretical calculations, it has been observed that the reaction proceeds through a product like transition state, with maximum stabilization from the hyperconjugation effect of methyl groups in 2-methyl-1,3-dioxolane.

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Mg^{2+}-DOPING INDUCED MODULATION OF ULTRAFAST EXCITON DYNAMICS IN $FAPbBr_3$ NANOCRYSTALS

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Introducing dopants into perovskite nanocrystals has proven to be an effective method for modifying their optical and electronic properties for advanced optoelectronic applications [1]. This study explores the synthesis, characterization, and photophysical properties of magnesium Mg^{2+}-doped $FAPbBr_3$ perovskite nanocrystals. By embedding Mg^{2+} ions into the $FAPbBr_3$ lattice, we aim to boost photoluminescence efficiency through radiative decay engineering. Morphological analysis via PXRD, XPS, and FETEM reveals that doping causes lattice contraction (from 12 nm to 10 nm), resulting in increased confinement. Mg doping (4.8%) enhances photoluminescence intensity and quantum yield (increasing from 60±3% to 75±3%), along with a higher radiative recombination rate (2.35 times that of undoped nanocrystals). In femtosecond transient absorption experiments, excitation at a wavelength (λ_{ex} = 400 nm) much higher than the nanocrystals' band gap (520 nm) generates hot excitons [2]. The hot-carrier cooling time in undoped nanocrystals is 1094 ± 45 fs, while in the doped system, it is significantly faster (710 ± 26 fs) due to the enhanced coupling of conduction band states with the dopant states (Figure 1). The reduction of trap states and increased trapping-detrapping rate with doping contribute to a faster ground-state bleaching (GSB) recovery [3]. These results offer new insights into doping strategies for perovskite nanocrystals and pave the way for developing high-performance optoelectronic materials

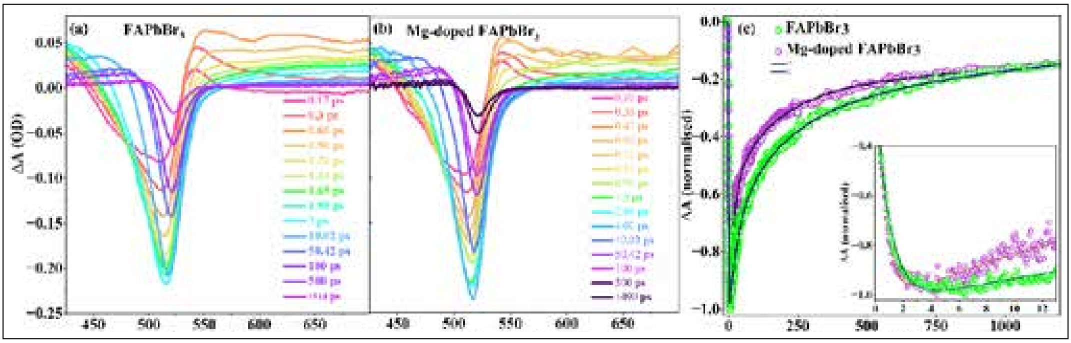

Figure 1. TAS of (a) $FAPbBr_3$ and (b) Mg^{2+}-doped $FAPbBr_3$. (c) Comparison of GSB recovery kinetics of doped and undoped $FAPbBr_3$, inset depicts the shorter timescale.

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ULTRAFAST INSIGHTS FULL-COLOUR LIGHT-EMITTINGC-DOTS TO REVEAL THE CORE AND SURFACE STATEHETEROGENEITY DURING ELECTRON TRANSFER

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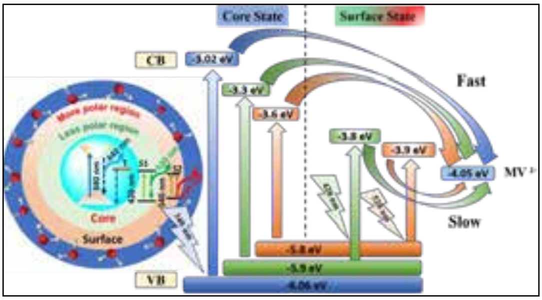

Figure 1. Schematic representation of different relaxation pathways of C-Dots in the presence of MV^{2+} after selective exaction from core and surface state.

Designing the Carbon dots (C-Dots) with controlled optical properties has been a persistent challenge due to their complex structural diversity. To explore themystery of C-Dots, three different C-Dots (blue, green, and red-emitting) were synthesized from the same starting materials using hydrothermal methods and separated by silica column chromatography. Despite varying excitation dependent emission properties, all purified C-Dots with same size and interplanar spacing (~4 nm, ~0.21 nm)exhibited uniform emission maxima. The investigation of carrier dynamics revealed that graphitic nitrogen in the core and oxygen-containing functional groups at the surface predominately influence their emission properties. Further, the heterogeneity of core and surface state of C-Dots during electron transfer (ET) was investigate via steady-state, time-resolved fluorescence, and ultrafast transient absorption spectroscopy and revealed that the core state has a stronger electron transfer (ET) ability than the surface state. The surface states are hindered the ET process due to the oxygen-containing surface groups which actas an electron scavenger. The graphitic nitrogen in the core and oxygen groups on the surface contribute to the distinct ET behaviour infull-colour light-emitting C-Dots, providing the new insights for the designing of metal-free and light-harvesting systems..

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PYRANO[3,2-C] CHROMENE BASED SENSOR FOR DETECTION OF MICROBIAL AND HUMAN CONTAMINATION IN ENVIRONMENTAL SAMPLES

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Dissolved organic matter (DOM) in water bodies serves as a important indicator of ecosystem health. Fluorescence spectroscopy has emerged as a sensitive tool for analyzing DOM content in water. The presence of amino acids can directly indicate microbial activity or human waste contamination [1]. However, many amino acids are non-fluorescent, and the few that are fluorescent, such as tryptophan, tyrosine, and phenylalanine, typically exhibit low fluorescence quantum yields, which can limit their detection sensitivity. Hence a probe capable of detecting amino acids has much potential in the quantitative as well as qualitative analysis. In this regard, A new pyrano[3,2-C]chromene derivative, 2-amino-4-(4-chlorophenyl)-4,5-dihydro-5-oxopyrano[3,2-C]chromene-3-carbonitrile, has been synthesized via a one-pot multicomponent reaction, utilizing micro wave irradiation.

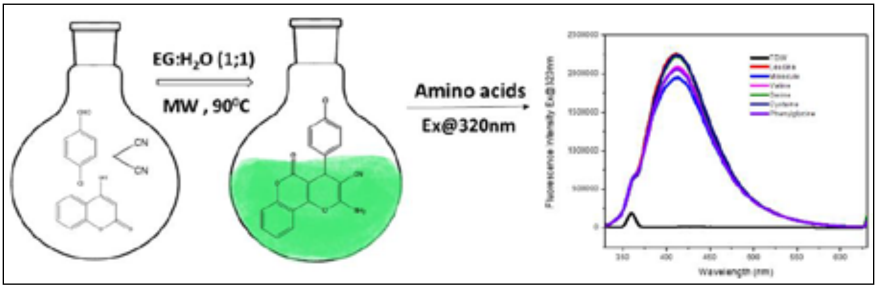

Figure 1. One pot synthesis of pyrano[3,2-C]chromene-based molecule for the selective detection of amino acids in real samples

Fluorescence spectroscopy data confirms that the synthesized probe selectively detects amino acids through a fluorescence enhancement mechanism. This probe is highly selective and have comparable analytical figures of merits, LOD and LOQ values of 0.08 µM and 0.25 µM respectively. It has minimal interference from metal ions and other quenchers/enhancers, aiding in the identification of microbial and human contaminants in water.

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CHARGE CARRIERS DYNAMICS IN $CsPbBr_3$-PbSe EPITAXIAL NANOCRYSTAL HETEROSTRUCTURES

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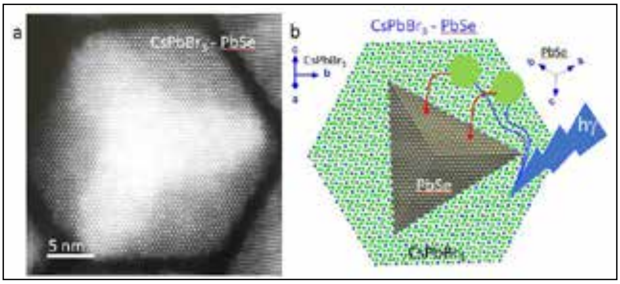

Figure 1. (a) HAADF-HRSTEM images of $CsPbBr_3$-PbSe heterostructure. (b) Atomic model of $CsPbBr_3$-PbSe heterostructure showing carrier transfer $CsPbBr_3$ to PbSe.

Lead halide perovskite and chalcogenide heterostructures that share the ionic and covalent interface bonding might be the possible materials for bringing surface stability and superior photo responsivity to these emerging perovskites nanocrystal. However, in spite of significant successes in the development of halide perovskite nanocrystals, their epitaxial heterostructures and their exited state dynamics with appropriate chalcogenide nanomaterials largely remained unexplored [1]. Keeping the importance of these materials in mind, herein, the epitaxial heterostructure of cubic PbSe with two different faceted orthorhombic $CsPbBr_3$ nanocrystals are reported. These are synthesized following the standard classical approach of heteronucleations of chalcogenide PbSe with $CsPbBr_3$ perovskite nanostructures [2]. With ultrafast transient absorption studies, the charge carrier dynamics of $CsPbBr_3$-PbSe as compared to the $CsPbBr_3$ are also established. As these are first of its kind nanostructures that are obtained with epitaxial growth of chalcogenides on halide perovskites, this finding is expected to pave the way for designing other heterostructures and studying their charge carrier dynamics.

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SYNTHESIS OF 4-AMINOPHTHALIMIDE (4-AP) DERIVATIVES AND ITS PHOTOPHYSICAL PROPERTIES

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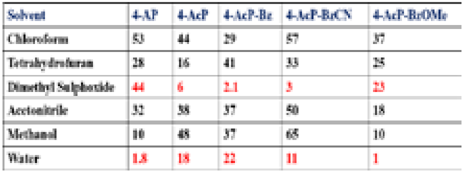
4-5-6-7-8-Aminopthalimide (4-AP) is a well-known fluorescent probe with high quantum yield, fluorescence lifetime [1] and photo stability due to which it finds applications in sensing microenvironment, metal ions and other aromatic nitro compounds. Although it has excellent photo physical properties, it does not exhibit any solid as well as aggregated state fluorescence which restricts its application in the field of optoelectronics and drug delivery. In the present work, we have synthesized four 4-AP derivatives with appreciable solid as well as aggregated state fluorescence by retaining its all other solution state photo physical properties [2]. By substituting one of the amine protons with amide group (4-AcP) and keeping it as control unit, we studied the excited state properties/processes by substituting the phthalimide proton with benzylic (4-AcP-Bz) group having cyano (4-AcP-BzCN) and methoxy (4-AcP-BzOMe) substitution at para positions by simple condensation technique. Steady state and time resolved fluorescence measurements have been carried out to understand the photo physical properties of the synthesized derivatives. AIEE studies exhibits ~3 to 10 fold increment in the fluorescence of these derivatives in the aggregated state when compared with the monomeric solution. Metal ion sensing behaviour of all the synthesized derivatives were investigated. Although all these 4-AP derivatives have remarkable selectivity towards Fe^{3+} ion detection, 4-AcP-Bz turns to be more significant as it has a detection limit of 0.07 µM in water for Fe^{3+} ions, which facilitates its sensing performance in real time detection. Furthermore, interference studies reveal its greater tolerance towards other ions. To summarize, this work highlights the usage of 4-AP derivatives in wider range of applications.



Solvent	4-AP	4-AcP	4-AcP-Bz	4-AcP-BzCN	4-AcP-BzOMe
Chloroform	53	44	29	57	37
Tetrahydrofuran	28	16	41	33	25
Dimethyl Sulphoxide	44	6	2.1	3	23
Acetonitrile	32	38	37	50	18
Methanol	10	48	37	65	10
Water	1.8	18	22	11	1

Table 1 : Quantum yield of 4-AP and its derivatives in different solvents (highlighting the increment in quantum yield in case of its aggregated form)

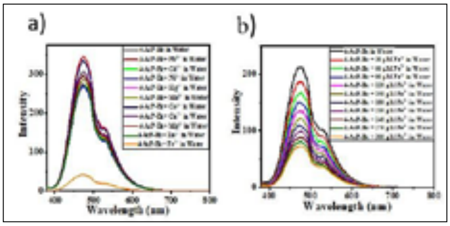


Figure 1. Selectivity (a) and sensitivity (b) of 4-AcP-Bz towards Fe^{3+}

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SYNTHESIS AND CHARACTERIZATION OF TYROSINE STABILIZED SILVER NANOCLUSTERS AND ITS ANTICANCER ACTIVITY

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Synthesizing atomically precise nanoclusters (NCs) is an emerging area of material science. NCs are gaining attention due their exceptional physical and chemical properties. However, they present several synthetic and characterization challenges, calling for designing a robust and reproducible synthesis pathway.

Present study revolves around optimizing parameters like pH, temperature and metal to ligand ratio for efficient synthesis of fluorescent tyrosine stabilized silver nano-clusters (Tyr-Ag NCs).

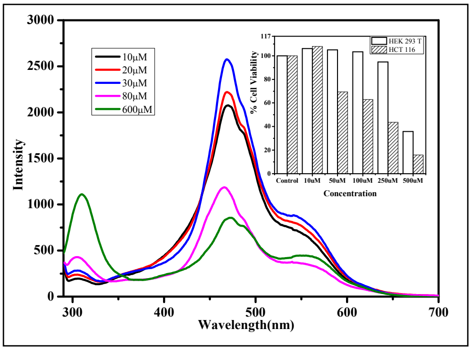

Figure 1. Emission Spectra of varied concentration of Tyr, $[Ag^+]$=100mM, pH=11, Temp=80°C,t=Day 3. Inset: Effect of Ag NCs on Cell viability of HEK 293T and HCT 116.

Spectrophotometric studies were carried out to understand the interaction between silver and amino acids, thereby optimum metal to ligand concentration was found to be 30 and 300μM, respectively which showed higher emission intensity as depicted in fig 1. Optimized temperature and pH for the synthesis was 80 °C and 11, respectively. The characterization of fluorescent yellow nano-clusters demonstrated absorption spectra in UV-Vis spectroscopy at 416nm and emission maxima at 469 nm. Further, the as-synthesized Tyr-Ag NCs were characterized by DLS and TEM to determine morphology and size. The binding affinities were studied by cyclic voltammetry. Inset shows the absence of cytotoxicity against normal cell line (HEK 293T) confirming biocompatibility of the Tyr-Ag NC. The cytotoxicity assay on colon cancer cell line (HCT 116) showed IC_{50} value around 200μM.The bio-imaging and fluorescent properties of the material will be presented in detail.

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EFFICIENCY OF ENCAPSULATION OF THIOFLAVIN T (ThT) INTO DIFFERENT BILE SALT AGGREGATES: A FEMTOSECOND FLUORESCENCE STUDY

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Although bile salts are amphiphilic compounds, their structure differs significantly from that of other typical surfactant molecules. The structure possesses a hydrophobic convex surface and a hydrophilic concave surface. Hydrophobic interactions between monomers form primary aggregates above the critical micellar concentration. These primary aggregates undergo hydrogen bonding and hydrophobic interaction at extremely high concentrations to generate secondary aggregates. A distinctive feature of these aggregates is their possession of both hydrophilic and hydrophobic pockets, enabling them to bind various guest molecules based on their characteristics. In this study, we examined the binding affinity of the amphiphilic probe Thioflavin-T (ThT) in three distinct bile salt aggregates: Sodium Cholate (NaCh), Sodium Taurocholate (NaTC), and Sodium Deoxycholate (NaDC). The variations in the absorption and emission characteristics of the probe molecule (ThT) were observed to be responsive to the rise in respective bile salt concentration. The encapsulation of ThT by bile salt aggregates leads to a substantial increase in both the emission intensity and emission maxima. Furthermore, we have examined the impact of modified ionic strength of the medium on the spectroscopic characteristics of ThT within bile salt aggregates by introducing sodium chloride (NaCl). The fluorescence lifespan of ThT in bile salts is greatly enhanced in the presence of NaCl, mostly because of the subsequent development of more rigid aggregates. Using iodide (I–) as an external ionic quencher, the encapsulation effectiveness of ThT in bile salt aggregates has been evaluated. Our result indicates that NaDC aggregates exhibit greater efficacy in modifying the photophysical characteristics of ThT compared to the other two bile salt aggregates.

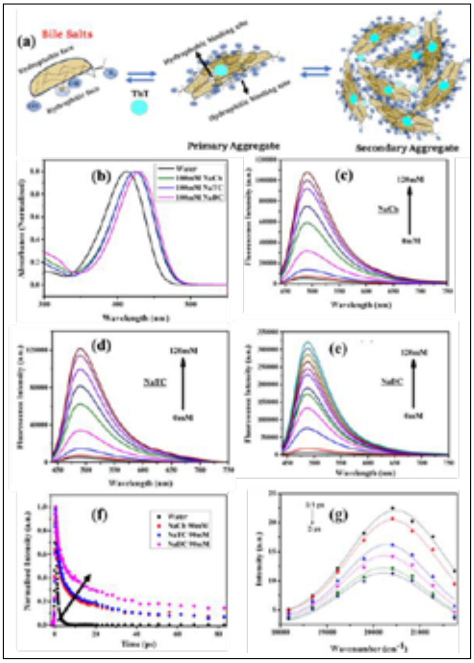

Figure 1. ‘a’ denotes general structures of monomers and different aggregates of bile salts. ‘b-g’ represents various spectroscopic properties of ThT inside different bile salt solutions.

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PHOTOCATALYTIC REACTION OF L-TYROSINE IN THE PRESENCE OF COLLOIDAL CdS

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A colloidal solution of cadmium sulfide (CdS) was prepared by the method described by Spanhel et al. [1]. Cadmium iodide and sodium sulfide were used as precursors and sodium hexametaphosphate as a stabilizing agent. The synthesized colloidal CdS was characterized by Transmission Electron Microscopy (TEM) and X-Ray Diffraction (XRD) measurements. The particle size of the photocatalyst was found to be 9 ± 2 nm from TEM analysis. The photocatalytic reaction of L-tyrosine in the presence of colloidal CdS was investigated by using UV-visible spectroscopy. A 150 W tungsten lamp emitting light in wavelength range 400-720 nm was used as the irradiation source. L-tyrosine was found to undergo oxidation as a result of the photochemical reaction. Dopachrome was identified as one of the products using liquid chromatography-mass spectrometry (LC-MS) technique. A plausible mechanism for the oxidation of tyrosine by colloidal CdS was discussed in light of the present and previous findings reported by earlier workers [2].

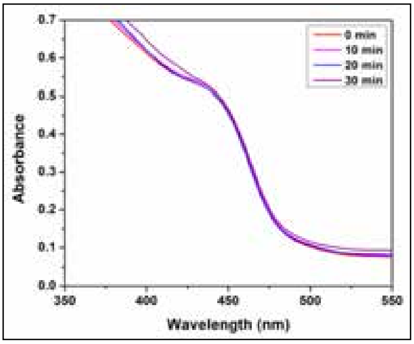

Figure 1. UV-vis absorption spectra of CdS and L-tyrosine as a function of irradiation time as indicated in the inset.

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STUDIES OF PHOTOPHYSICAL BEHAVIOR OF FLUORESCENT CATIONIC DYE IN CUBOSOMES: THEIR USE IN SENSING APPLICATIONS

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Cubosomes are biocompatible, nanostructured liquid crystalline carriers with a unique bicontinuous cubic phase morphology, formed through the self-assembly of amphiphilic lipids in specific ratios[1]. These nanoparticles exhibit reversed cubic phases and possess distinct physicochemical properties that render them a promising platform for drug and gene delivery [1]. Fluorescent molecules or materials are commonly employed for tracking cargo within drug delivery systems.The photophysical behaviour of fluorescent materialsin cubosomes remains relatively unexplored. Cucurbit[n]urils, macrocyclic oligomers consisting of glycoluril units linked by methylene bridges, are recognized for their high affinity towards neutral and cationic species [2]. We have explored the unique affinity of Cucurbiturils (CB[6]) and (CB[7]) towards developing various supramolecular sensors for spermine (SP) and spermidine (SPD) [3]. In the current project, we intended to use a monoolein derived cubosome-CB[7]-cationic dye nanoenzyme for the supramolecular detection of SP and SPD.Upon the addition of CB[6] and CB[7] to a solution containing cubosomes and a fluorescent dye, a significant reduction in fluorescence intensity was observed. This quenching effect is likely due to the preferential interaction of the dye with the cationic binding sites of the CB[6] and CB[7] within the cubosomal structures. The host-guest conjugate remains non-fluorescent. Subsequently, the fluorescence is retrieved upon the introduction of spermine (SP) and spermidine (SPD) into the sensing system, suggesting that CB[6] and CB[7] preferentially release the cationic dye and bind to SP and SPD.Thus, a sensitive supramolecular sensor is developed in this manner.

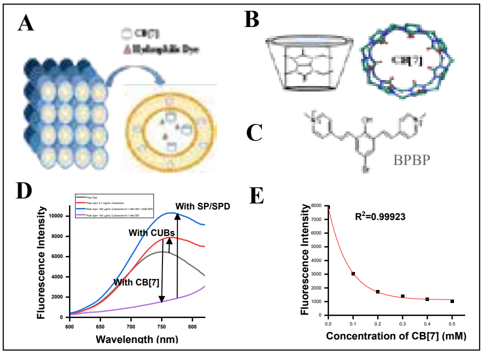

Figure 1. A) Representative structure of cubosome and possible interaction B) Structure of CB[7] C) Structure of cationic dye D), E)Fluorescence change upon the addition of each component of the supramolecular sensing system.

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DESIGNING OF FOUR SYSTEM FRET SERIES& ITS APPLICATIONS

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FRET (Förster Resonance Energy Transfer) systems are widely utilized to investigate the molecular dynamics and structural characteristics of complex molecules.[1] While much of the existing research has focused on two or three molecule FRET systems, this study aims to develop a three step FRET system. This innovative approach employs four distinct molecules that exhibit significant overlap in their electronic spectra, allowing for the validation of its efficiency through both two-step and three-step FRET processes.

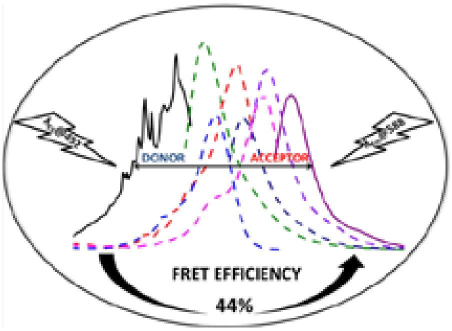

Figure 1.Pictorial representation of FRET series with four systems their efficiency.

The theoretical framework for analysingmultiple energy transfer events between donors and acceptors is established through the following equation (FRET relay),

$$E_{relay} = I_4/\tau_4 = E_{12} * E_{23} * E_{34} \text{ where } \tau_4 = \frac{1}{(K_{r_4} + K_{nr_4})}$$

and subsequently verified using experimental data. Ultimately, this advanced FRET system is applied across various applications, demonstrating its versatility and effectiveness.

The primary application of this research is to develop a cost-effective yet efficient anti-counterfeiting measure. While there has been extensive work on creating anti-counterfeit solutions using quantum dots, some of which incorporate the FRET concept [2], this study focuses on designing a novel series of readily available molecules. By leveraging these common materials, we aim to create effective anti-counterfeiting measures that open up new possibilities for practical applications in security and authenticity verification.

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DESIGN AND APPLICATION OF FLUORESCENT PURINE PROBE FOR ER IMAGING AND STRESS MONITORING

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The endoplasmic reticulum (ER) is central to maintaining cellular homeostasis, playing key roles in protein folding, lipid metabolism, and calcium regulation. Disruptions in ER function can lead to ER stress, a condition that activates the unfolded protein response (UPR) to restore balance. If ER stress is prolonged, however, it can contribute to pathological conditions such as neurodegeneration, cancer, and metabolic disorders. Given the critical role of ER stress in health and disease, there is a pressing need for tools that enable precise, real-time monitoring of ER stress dynamics. In this work, we present the design, synthesis, and characterization of two novel fluorescent probes: purine phenothiazine (PP) and aminopurine phenothiazine (AP). Investigation of the cellular imaging reveals selective ER localization and sensitivity to ER stress conditions. Notably, the PP probe exhibited strong localization within the ER, making it an invaluable tool for studying ER-associated processes. In contrast, the AP probe, despite its structural similarity to PP, displayed reduced specificity, underscoring the importance of subtle molecular modifications in targeting intracellular compartments.

Biological evaluation of these probes under ER stress-inducing conditions, such as nutrient starvation and tunicamycin treatment, revealed that the PP probe selectively accumulates in the ER and provides real-time, spatially resolved detection of ER stress.

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ULTRAFAST ENERGY TRANSFER AND ELECTRON TRANSFER DYNAMICS IN TETRARYLPYRROLO[3,2-*b*] PYRROLE-BODIPY DYADS

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Photo induced energy transfer (EnT) and electron transfer (eT) events in molecularly coupled chromophores play important role in artificial light harvesting materials relevant to optoelectronic and photocatalytic application. In depth understanding of energy transfer and electron transfer is crucial for development of superior light harvesting materials. In this study, we explored ultrafast photo induced energy and electron transfer events in a molecular dyad comprises of tetraarylpyrrolopyrrole (TAPP) donor and a boron dipyrromethane (BODIPY) acceptor connected by phenylethynyl spacer (Figure 1). Femtosecond resolved transient absorption and transient fluorescence were monitored to unravel solvent dependent excited state dynamics of the dyad.

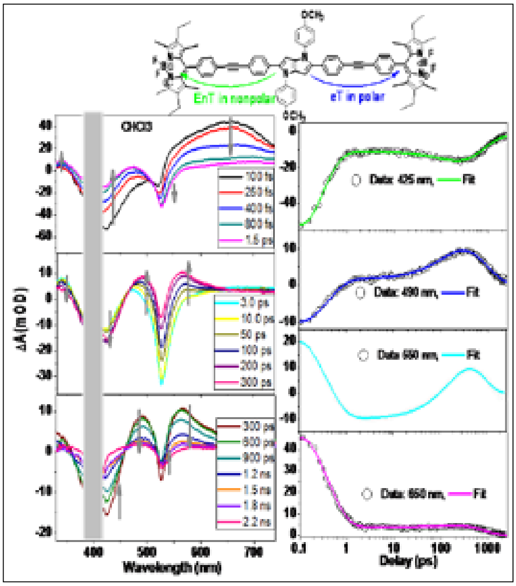

Figure 1. Molecular structure of the dyad and ultrafast transient absorption dynamics in chloroform.

In non-polar solvent (such as cyclohexane and toluene), purely energy transfer dynamics (τ ~450 fs), from TAPP to BODIPY govern the excited state dynamics of the dyad which could be fully accounted by Forster resonance energy transfer mechanism [1]. However, in medium polar solvent (such as chloroform), ultrafast energy transfer ((τ ~480 fs) is followed by slow electron transfer (τ ~200 ps) (Figure 1). In polar solvents, energy transfer and electron transfer dynamics compete in early timescale (<300 fs) followed by complete electron transfer in a few picosecond timescales. Competing energy and electron transfer dynamics were distinguished by excitation wavelength dependent transient absorption experiments. Ultrafast fluorescence up-conversion experiment further unravelled distinct electron transfer kinetics from donor and acceptor excited state which occurs in different time regime due to difference in driving force of electron transfer process. Solvent polarity and excitation wavelength dependent electron transfer dynamics was fully rationalized by Marcus theory of electron transfer.

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ULTRAFAST ANTI-AROMATICITY RELAXATION DYNAMICS IN p-DIACETYLPHENYLENEDIAMINE - A SMALLEST RED LIGHT EMITTER.

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Recent studies showed that a tiny single-benzene fluorophore compound, p-diacetylphenylenediamine (p-DAPA), exhibits an unusually large Stokes' shift (4570 cm^{-1}) and emits at the red region of the visible spectrum (618 nm)[1]. Hence, to understand this unique photophysical characteristic, we have investigated detailed spectroscopic properties of p-DAPA using steady-state and time-resolved spectroscopic methods in different classes of molecular solvents. The steady-state measurements revealed negative solvatochromism of p-DAPA in polar solvents suggesting relatively more stabilization of the ground state than its excited state. The Stokes' shift is found to be significantly higher in protic solvents as compared to aprotic solvents with comparable dielectric constant. The linear correlation between the Stokes' shift and the hydrogen bond donating ability parameter (α) for protic solvents indicates the role of H-bonding in the observed large Stokes' shift in p-DAPA. Femtosecond transient absorption (FSTA) measurements were performed to understand the role of α on the excited state dynamics of p-DAPA. Irrespective of the nature of the solvent, FSTA data shows a strong excited state absorption (ESA) band and a stimulated emission (SE) band as shown in Figure 1. The dynamics of both ESA and SE bands are largely affected by the hydrogen bond donating ability of the solvent. In all solvents, the ESA and SE bands show an ultrafast growth component. [1]Considering the fact that the photoexcitation results in the anti-aromaticity in the benzene core of p-DAPA, growth component in FSTA measurements was assigned to such anti-aromaticity in its excited state. The rate of anti-aromaticity relaxation is seen to increase with the increase in α value of protic solvents. The time constant for the excited state anti-aromaticity relaxation varies from 0.6 ps in water to 8 ps in acetonitrile (ACN). Thus, it can be inferred that the transition of the anti-aromatic state to the aromatic state is highly affected by the solute-solvent H-bonding. Such mechanistic details are very useful in tailoring new organic light emitter compounds.

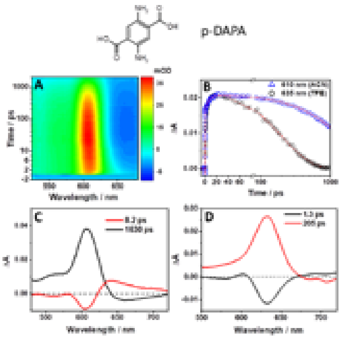

Figure 1: (A) Colour map plot of the transient absorption data of p-DAPA in acetonitrile (ACN). (B) Decay kinetics of ESA in ACN and 2,2,2-trifluoroethanol (TFE). Decay associated spectra in ACN (C) and TFE (D).

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Organisers acknowledge the financial support from

Board of Research in Nuclear Sciences (BRNS)

and

Anusandhan National Research Foundation (ANRF)

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