

ABSTRACT BOOK

**20th National Conference on Surfactants, Emulsions and Biocolloids
NATCOSEB-XX
9 - 11 December 2021**

**a virtual
conference**

**organized
by**

**Department of Chemistry
Indian Institute of Technology Guwahati**

in association with

Indian Society for Surface Science and Technology, Kolkata

Patron

Prof. T. G. Sitharam
Director, IIT Guwahati

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26 November 2021

Message from Director, IITG

I am very glad to know that the 20th edition of National Conference on Surfactants, Emulsions and Bio-colloids (NATCOSEB) of the Indian Society for Surface Science and Technology (ISSST) is being organized in an online mode by Department of Chemistry, Indian Institute of Technology, IIT Guwahati during 9-11th Dec 2021.

The Indian Society for Surface Science and Technology (ISSST) is an organization for the cultivation, interaction and dissemination of knowledge in the field of colloids, surface science and technology. It also strives to promote Industry-Academia interaction. The NATCOSEB series of conferences brings together eminent researchers from the highly interdisciplinary area from all over the country to explore the recent advancements in the fundamental and applied areas of colloids and surface science. This series promotes a stimulating environment for intense scientific discussions, exchange of ideas and development of collaborations among the scientific peers across the country.

Colloids are mixtures of one substance forming microscopic insoluble particles (dispersed phase) scattered uniformly in the other substance (dispersion medium). Though according to one school of thought colloids should have a liquid dispersion medium, other school of thoughts even include aerosols and gels as colloids. The area is highly interdisciplinary and finds various interesting applications in food industries, environmental remediation, material science and bio-medical fields.

It's extremely encouraging to know that eminent scientists from all over India are participating in NATCOSEB-XX. I sincerely believe that this conference will provide a platform for the emergence of new ideas and concepts that will cross boundaries and promote science that will create a better future for the society.

I wish the conference all the best.

(T. G. Sitharam)

Message from the President, ISSST



Prof. Dr. Asit Baran Mandal
FASc., FRSC (UK), FNAE, FSAB (Hony.),
INAE Distinguished Professor
(Formerly Director and Outstanding Scientist,
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CSIR-CGRI



Message

Dated: 01st December, 2021

The biennial National Conference on Surfactants, Emulsions and Biocolloids (NATCOSEB) of Indian Society for Surface Science and Technology (ISSST) aims to provide a platform to scientists, technologists and researchers for exchanging their ideas and advancement through scientific discussion. The participants are expected to communicate among themselves on their studies on micelles, emulsions, microemulsions, gel, monolayer, nanomaterials and nanotechnology, polymers and biopolymers, soft matter, biocolloids and biomimetic systems, supramolecular assemblies and various other aspects of surface science. The ISSST was established in 1983 at Jadavpur University, Calcutta with the aim to cultivate and disseminate the knowledge of surface science among researchers, students, teachers and general public. I must mention here my good old days when I was a student of Jadavpur University doing PhD in the field of Micellar and Mixed Micellar Systems under the guidance of eminent Professor S. P. Moulik, I had the opportunity to read an article by Prof. P. Mukherjee entitled "The wide world of Micelles", which was justified by Prof. Mukherjee. He mentioned in that article that when the pioneering works of micelles of McBain submitted to Royal Society of London, it was rejected by the chairman of Royal Society in two words: "Nonsense McBain". Although it was disheartening to McBain, subsequently the concept of Micelle was accepted with the advent of Light Scattering, magnetic resonance spectroscopies and many other sophisticated techniques. I understand Prof. J.W. McBain was the Founder Director of National Chemical Laboratory (NCL), Pune and Visiting Professor at the Stanford University, USA. According to some physicists, chemists and biologists, it may be appeared that surface science is superficial in nature, but in the true sense, it is not: Many reactions take place on the surface and even in the core of the micelles simultaneously in the fast and slow processes and exchanged thereby. Therefore, the importance of surface science can not be ignored. The industry-academia collaboration is one of the stated goals owing to the importance of surface science in general public life. Society organizes international, national and local seminars throughout the year and it has more than 600 members from India and abroad. The society also publishes a peer reviewed international research journal: Journal of Surface Science and Technology (JSST) as well as a Newsletter. Recently, an unique article by Profs. A. K. Rakshit and S. P. Moulik has appeared in JSST in view of the completion of 100 years in surface science around the world.

Whereas Indian Institute of Technology Guwahati, the sixth member of the IIT fraternity was established in 1994, one of the premier academic institutions located in North Eastern region of our country. As the cutting edge research today has become more of a group and collaborative (Team-Spirit) was rather than individual effort, the ISSST hopes that NATCOSEB will help the researchers to bond among themselves for the betterment of their own research and also for the benefit of the society at large. I am happy that **this year NATCOSEB 2021 being organized by IIT Guwahati, Assam under the aegis of Indian Society for Surface Science and Technology, Jadavpur University, Kolkata during December 9-11, 2021 on online** because of the Covid-19 pandemic situation. In addition to prestigious Prof. B. N. Ghosh memorial and Dr. Shyamasri Gupta memorial awards, the Key Note and Plenary lectures and many invited lectures by the eminent scientists, Oral and Posters presentations by the young students would be presented during this conference. Prof. S. Aditya, the Founder President of ISSST has passed away recently and Prof. A. C. Dash has generously donated some money to ISSST this year to institute an award in honour of Prof. Aditya and the above award will be given to the student for the best oral presentations during this conference. The former presidents viz., Profs. D. K. Chattoraj, S. P. Moulik and A. K. Rakshit are constantly supporting us throughout and they wish our conference a grand success. Therefore, it gives me a great pleasure to write this message and I congratulate both ISSST and IIT-G for organizing NATCOSEB-2021 and in the days to come, such initiatives and programs, which will benefit the industry, academic institutions and society at large.

Prof. Asit Baran Mandal

President, Indian Society for Surface Science & Technology
Jadavpur University, Kolkata.

Message from the Secretary, ISSST

INDIAN SOCIETY FOR SURFACE SCIENCE AND TECHNOLOGY JADAVPUR UNIVERSITY



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Ref. No.....

Date.....

3rd December, 2021

This is my honour to share my feelings with you about the Indian Society for Surface Science and Technology (ISSST). I am delighted to note that a joint venture of ISSST and Department of Chemistry, I.I.T., Guwahati in organizing a National Conference on Surfactants, Emulsions and Biocolloids (NATCOSEB – XX) would come into reality during December 9 – 11, 2021. The 20th NATCOSEB will attract the scientists in the field of Soft matter, biocolloids and biomimetic systems. The series of conferences in the field of surfactants is organized all over the world. The biennial NATCOSEB is the flagship conference of ISSST which provides a platform to scientists, technologists and researchers to exchange their ideas and advancement. This conference covers broad topics on self-aggregation of surfactants and the interfacial phenomena, new materials at interfaces, surface coatings, pharmaceutical and medicinal aspects.

I am confident that participants will enjoy hearing lectures from eminent personalities on the relevant fields and we all will be enriched. I personally believe that scholars will utilize this platform at their best.

I am sure that the conference will have a grand success.

Soumen Ghosh
Soumen Ghosh

Secretary, ISSST

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Foreword

It is a pleasure to welcome all the delegates to the 20th National Conference on Surfactants, Emulsions and Biocolloids (NATCOSEB-XX) being held during 9-11 December 2021. The conference is organized by the Department of Chemistry, Indian Institute of Technology Guwahati in association with Indian Society for Surface Science and Technology (ISSST), Kolkata. ISSST is one of the oldest societies in the world that focuses on surface science. Over the last several decades, the society with their continuous effort has made surface science popular in the country. We feel proud to be associated with the society and it is a pleasure to organize the conference in this department.

The aim of NATCOSEB-XX is to provide a common platform for showcasing the recent developments in the frontiers of surface, colloids, self-assembly and allied fields. Over the years, these subject areas are becoming more and more interdisciplinary in nature, with applications in many areas having industrial and societal impact, such as, nano-materials, biomedical and bioengineering, polymer, waste managements to name a few. A glance through this book of abstracts will definitely justify the depth of the advanced research in the present time. The NATCOSEB-XX proceeding will consist of Keynote Lecture, Plenary Lecture, Invited Talks, Students' Oral Presentations, Industrial Lecture and Poster Presentations by around 75 delegates. Moreover, there are some more lectures by the selected awardees for different awards. We are sure that the conference will provide a stimulating environment for intense discussions and exchange of ideas among the researchers for new collaborative and interdisciplinary research attempts on surface science as a whole.

Unfortunately, we are not in a position to welcome you in person due to the ongoing pandemic world-wide. The COVID-19 opened up a new way to learning and that is, "online". This is a new era and we are changing our habits constantly to cope up with the situation. Following the time's demand, for the first time, NATCOSEB is being organized virtually. This has not only reduced the number of lectures and the overall volume of the conference, most importantly, we all will miss the discussions during the poster sessions. Nevertheless, we have arranged a continuous poster session where videos recorded by the presenters are available to watch all the time. Moreover, the presenters can also be contacted through e-mail to clarify/discuss about any doubts/suggestions. Additionally, a live streaming of the conference on youtube.com will be available for any interested person to watch.

Sincere thanks to ISSST for their invitation to host the conference. We also want to take the opportunity to thank Prof. T. G. Sitharam, Director, IIT Guwahati for being the patron for this conference and his constant support. Thanks is also due to all faculty members of the department for their support. Special thanks to ChemCommun, RSC for sponsoring the student awards. We also want to thank our other sponsors, Aimil Limited and Anton Par for financial supports. Once again, we wish all the delegates a fruitful scientific endeavour.

Guwahati
9th December 2021

Organizing Committee
NATCOSEB-XX

Scientific Program

| Day 1: Thursday, 9th December 2021 | | |
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| 14:30 – 15:00 | Inauguration <ul style="list-style-type: none"> • Welcome address by HOD, Department of Chemistry, IIT Guwahati • Address by the Secretary, ISSST • Address by the President, ISSST • Address by the Guest of Honour, Director, IIT Guwahati • Vote of thanks by the convenor | |
| 15:00 – 15:40 | Plenary lecture (<i>Chair: Prof. Manabendra Ray</i>) | |
| | Prof. Amitava Das | Guanidinium Derivatives as Cationic C ₃ -Symmetric Gelators: Counter Anion Induced Chirality and Li-ion |
| Session Break | | |
| 15:50 – 16:20 | IL-1 Dr. Ketan C. Kuperkar | Self-Assembly and Micellar Transition Induced in Cationic Surfactant-Additive System |
| 16:20 – 16:50 | IL-2 Prof. Nand Kishore | Drug Partitioning in Colloidal Self Assemblies: Correlation of Structure-Property-Energetics Relationships |
| 16:50 – 17:20 | IL-3 Dr. Sangita Roy | Minimalist Peptide Engineering at the Nanoscale for Applications in Healthcare |
| 17:20 – 17:35 | OP-1 Mr. Arnab Banerjee | Hydrodynamic and Conformational Characterization of Aqueous Sodium Alginate Solutions with varying Salinity |
| 17:35 – 17:50 | OP-2 Mr. Arpan Mal | Interaction of the Heme Protein (Myoglobin) with Sodium Salts of Cholic and Deoxycholic acids in Phosphate buffer: A Detail Physicochemical and Molecular Docking Investigation. |
| 17:50 – 18:05 | OP-3 Mr. Manas Barai | Micro-Structural investigations on Oppositely Charged mixed Surfactant gels with Potential Dermal Applications |
| Day 2: Friday, 10th December 2021 | | |
| 15:00 – 15:40 | B. N. Ghosh Memorial Lecture (<i>Chair: Prof. K. P. Das</i>) | |
| | Prof. T. S. Pal | Surface Enhanced Raman Scattering (SERS) for Chemical Analysis |
| 15:40 – 16:20 | IL-4 Prof. Pralay Maiti | Control Drug Delivery for Better Healthcare |
| 16:20 – 16:50 | IL-5 Dr. Uttam Manna | Michael Addition Reaction for Achieving Durable Bio-inspired Liquid Wettability |
| 16:50 – 17:05 | OP-4 Ms. Oindrila Biswas | Transmembrane Cl ⁻ /HPO ₄ ²⁻ Antiport Activities of 2-Benzimidazolylthiourea Receptors. |
| 17:05 – 17:20 | OP-5 Ms. Payel Dowari | Artificial Hydrolase: Systematic Development and Immobilization on Silica Surface for Enhancement of Activity, Enantio-Selectivity and Reusability. |

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| 17:20 – 17 | OP-6 Ms.Shikha Ayeri | Smart Microgel-Stabilized Pickering Liquid Crystal-in-Water Emulsions and their Response. Towards Amphiphiles |
| 17:35 – 17:55 | JSST Best Paper award lecture Dr. Sathish Sundararaman | Evaluation of E-Fenton Process in Decolourization of Azo Dye (Congo Red) and its optimization studies using RSM |
| 17:55 – 18:10 | Industrial Lecture Dr. Rishi Gupta | Dynamic Light Scattering (DLS) and Electrophoretic Light Scattering (ELS) Technique and Application |
| Day 3: Saturday, 11th December 2021 | | |
| 15:00 – 15:30 | Syamasi Gupta Award Lecture (<i>Chair: Prof. Amiya Panda</i>) | |
| | Prof. Debapratim Das | Exploring the Possibility of Creating Life-Like Systems Using Supramolecular Peptide Amphiphiles |
| 15:30 – 16:00 | IL-6 Dr. I. Mukherjee | Encountering Emulsion formation at Oil Production and Processing Units (up and down stream) and smarter way of utilizing Emulsion Breaker (Demulsifier) chemistries at various Process Units. |
| 16:00 – 16:30 | IL-7 Dr. A. A. Dar | Triple-Mode Orthogonal Emission Color Tuning with White Light ON/OFF Switching from a Trimolecular Cocktail in Cationic Micelles for Prospective Anticounterfeitng Applications. |
| 16:30 – 17:00 | IL-8 Prof. S. S. Bhagwat | Fractional additions - Large property changes |
| 17:00 – 17:30 | IL-9 Dr. R. Verghese | Responsive DNA Nanostructures for Cancer Therapy |
| 17:30 – 18:00 | IL-10 Dr. Subhabrata. Maiti | Dynamic Modulation of Surface pH of a Catalytic Nanoparticle |
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Posters and corresponding videos will be available throughout the conference on <https://event.iitg.ac.in/natcoseb2021/>

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| OL-3 | Micro-Structural investigations on Oppositely Charged mixed Surfactant gels with Potential Dermal Applications <i>Mr. Manas Barai</i> |
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| OL-5 | Artificial Hydrolase: Systematic Development and Immobilization on Silica Surface for Enhancement of Activity, Enantio-Selectivity and Reusability <i>Ms. Payel Dowari</i> |
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| P-38 | A stimuli-responsive anticancer drug delivery system with inherent antibacterial activities <i>Subhasis Dey</i> |
| P-39 | Smart Thixotropic Hydrogels by Disulfide-Linked Short Peptides for Effective Three-Dimensional Cell Proliferation <i>Sumit Chowdhuri</i> |
| P-40 | Facets Dependent Catalytic Activity of Pd Nanocrystals for the Remedy of Organic Pollutant: A Mechanistic Study <i>Swarnalata Swain</i> |
| P-41 | Biodegradation of Waste Cooking Oil and Simultaneous Production of Rhamnolipid Biosurfactant by <i>Pseudomonas aeruginosa</i> P7815 in Batch and Fed-Batch Bioreactor Studies <i>Swati Sharma</i> |
| P-42 | Photophysical Investigation of a Sub-Micellar Triblock Copolymer-Cationic Surfactant Aggregate for Gold Nanoplate Synthesis <i>Tapas Pal</i> |
| P-43 | Developing Collagen Mimetic Ionic Complementary Peptide Hydrogels for Biomedical Applications <i>Vijay K. Pal</i> |
| P-44 | Self-Assembly and Micellar Transition in the Cationic Surfactant Triggered by the Alcohol <i>Vinod Kumar</i> |

A black and white photograph of a microphone on a stand, positioned in the lower-left quadrant. The microphone has a textured, mesh-like grille. The background is dark and out of focus, featuring several bright, circular bokeh lights that suggest a stage or lecture hall setting. The overall mood is professional and focused.

PLENARY LECTURE

Guanidinium Derivatives as Cationic C₃-Symmetric Gelators: Counter Anion Induced Chirality and Li-ion Conduction

Amitava Das



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A new class of cationic achiral C₃-symmetric gelator (having three pendant pyridine moieties) is found to self-assemble in MeOH/H₂O (1:1, v/v) solution. This lead to the generation of moderately strong gel. Interestingly, a counter anion exchange assisted approach is adopted to introduce a chirality signature, which is confirmed by circular dichroism (CD) spectroscopy as well as microscopic images.

Importantly, analogous tris-carboxy derivatives having a *three-fold* symmetry (**1**, **2** and **3**) undergo self-assembly processes to generate nanostructures. Compound **1** is found to self-assemble to produce a unique ordered rhombic dodecahedral shape in 1:3 DMSO-water (v/v) solvent system. The formation of the bulk nanocrystal with rhombic dodecahedral morphology could be explained in terms of the crystal facets and growth direction. Distinctly different self-assembled nanostructures are observed in 1:1 DMF-water (v/v) solvent system. The formation of self-assembled organic nanosheets (SONs) utilizing positional isomers of small organic molecules (**1**, **2** and **3**) is observed. The use of such SONs as solid state electrolytes (SSEs) for lithium-ion conduction at room temperature is examined. Solvent-assisted exfoliation of the bulk powder yields SONs, which display high crystallinity with an overall planner structure having the width of a few micrometres and thickness of a few nanometre range. Among these, SONs derived from isomer 2 is found to be most efficient for Li⁺-ion conduction.

Our recent efforts in understanding the unique aggregation behaviours of four different guanidinium ions derivatives and their implications shall be discussed in the presentation.

AWARD LECTUREs



B. N. Ghosh Memorial Lecture



Surface Enhanced Raman Scattering (SERS) for Chemical Analysis

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Raman Effect (1928) analytically exhibits inelastic scattering of incident light, a different kind of experience out of light-matter interaction. It was discovered using water even though theoretical background was already stimulated by mathematical equation due to Smekal (1923) but C. V. Raman experienced the novel scattering phenomenon for the 1st time. Then experimental discovery of laser made 'Raman Effect' perceptible as it is today. Thus elegance of vibrational spectroscopy truthfully gained solid ground and commercialization of the present day micro Raman instrument gives a truthful information. Then surface effect has made Raman scattering more sensitive and Raman Effect is raised to the occasion which is now known as surface enhanced Raman scattering (SERS). This serendipitous discovery relies largely on the type of laser, nature of a substrate and probe molecule. Instantaneously 'charge transfer effect' and 'electromagnetic effect' were put forwarded as the background theory to explain SERS effect which goes hand in hand till today to explains million times enhancement of some selected vibrational bands of a probe molecule. We have improvised several nanostructured materials, sometimes leaving aside conventional substrates, as effective SERS substrate. Thus importance of nanofabrication from 'bottom up' method expresses our manipulative skill. There 'hot spots' and 'blinking' take the analytical results almost to the single molecular level. Hope one day analysis would evade the laser selectivity and substrate specificity. That would be the real success story for SERS vis-à-vis Raman Effect.

Evaluation of E-Fenton Process in Decolourization of Azo Dye (Congo Red) and its optimization studies using RSM

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Recently there is a great focus on reusing/recycling the waste water in the dyeing process. The main objective of this research work is to effectively remove colour from textile wastewater using Electro Fenton (E-Fenton) process. E-Fenton process is the combination of Fenton and electrochemical processes. In this study decolorization of Congo red dye was investigated by E-Fenton process in a continuous reactor equipped with iron electrodes. Experiments were carried out in a reactor of working volume of 1L. The degree of decolourisation varies with the operating parameters. The optimal working conditions were maintained with an electrode potential difference of 2V, 40°C, pH 4. For Electro Fenton's process the parameters giving the highest efficiency were decolourisation percentage of 97%. The process parameters were optimized by using response surface methodology to understand the effectiveness of the interactions of variables when the maximum decolourization can be achieved. The experimental results proved that the combination of Fenton and Electrochemical process was an excellent method for treatment of textile wastewater.

Keywords: E-Fenton, Congo red, Azo dye, effluent, decolorization

AL-3

Syamasri Gupta Award Lecture

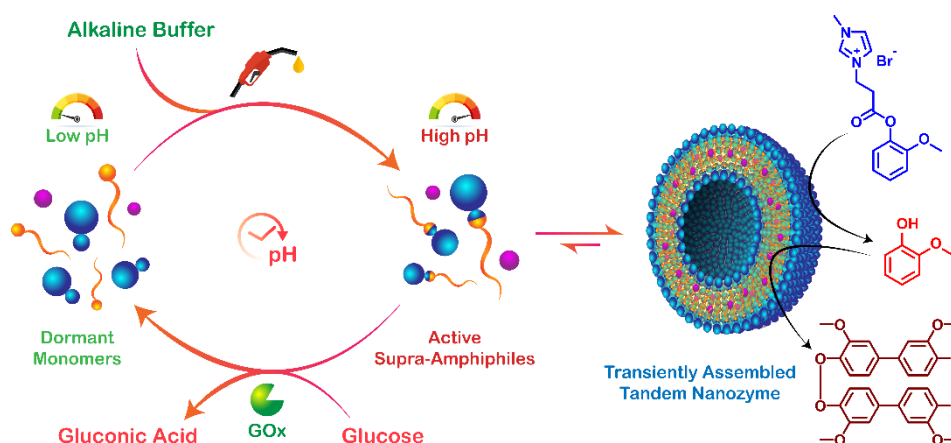
Exploring the Possibility of Creating Life-Like Systems Using Supramolecular Peptide Amphiphiles

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Natural out-of-equilibrium systems operate through a transient self-assembled state which formed with the help of a chemical fuel. However, this assembled state further loses its energy and returns back to its original non-aggregated form leaving a chemical waste. Constructing such transient systems synthetically is extremely challenging. Essentially, a combination of two opposite reactions is required where the rate of forward reaction should be faster than the backward reaction. Though creating such systems is an uphill task while on the other hand will open new vistas probably impacting modern science and technology enormously. We are in the process of developing such "Life-Like" systems using Cucurbit[8]uril assisted supramolecular amphiphiles (SPA) developed in our laboratory. In this lecture, I will talk about the formation of SPAs, utilization of the SPAs to develop fuel driven transient vesicles. Further, the lecture will cover the use of these transient vesicles to prepare transient tandem nanozyme.



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IL-1

Self-Assembly and Micellar Transition Induced in Cationic Surfactant-Additive System

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The study characterizes the micellization and shape transition induced in aqueous cetyltrimethylammonium bromide (CTAB) solution by the addition of the antioxidant: propyl gallate (PG) using tensiometry, rheology, and small-angle neutron scattering (SANS) techniques combined with the molecular dynamics (MD) simulation approach. The adsorption of CTAB at the air-water interface in the presence of varying concentration of PG revealed a progressive decrease in the critical micelle concentration (CMC), while the changes in different interfacial parameters indicated enhancement of the hydrophobicity induced by PG in the CTAB micellar system. The dynamic rheology behavior depicted the viscoelastic features in the investigated system while the small-angle neutron scattering (SANS) measurements depicted the existence of varied micellar geometry as a function of [PG] and temperature. The Density functional theory (DFT) simulation calculations and molecular dynamics (MD) provided an insight into the atomic composition of the examined system. Two-dimensional nuclear overhauser enhancement spectroscopy (2D-NOESY) showed the plausible location of PG inside the CTAB micelles. Various dynamic properties, viz., the radial distribution function (RDF), the radius of gyration (R_g), and solvent-accessible surface area (SASA), showed a significant microstructural evolution of the ellipsoidal micelles in the examined CTAB-PG system, where the changes in the micellar morphology with a more elongated hydrophobic chain and the increased R_g and SASA values indicated the notable intercalation of PG in the CTAB micelles.



Drug Partitioning in Colloidal Self Assemblies: Correlation of Structure-Property-Energetics Relationships

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Majority of synthetically developed new molecular entities or improved drug molecules have high hydrophobic content and low bioavailability. Therefore suitable drug delivery vehicles are required for effective delivery of the drugs at the target site. Self-assembled hydrocolloidal structures such as micelles, niosomes, and liposomes offer an effective environment for drug encapsulation. Literature information on drug encapsulation in such self assemblies has generally been qualitative in nature. We have quantitatively investigated the partitioning of a variety of drugs varying from antibiotic, anticancer, anti-inflammatory and antithyroid into self-assemblies of cationic, non-ionic and mixture of cationic and non-ionic surfactant micelles, as well as of niosomes and their interaction with the transport protein serum albumin upon subsequent delivery. Thermodynamic signatures accompanying the partitioning process [such as partitioning constant (K) and change in standard molar enthalpy (ΔH_m^o), standard molar entropy (ΔS_m^o), and standard molar free energy (ΔH_m^o)] have enabled a quantitative understanding of the role of functional groups on the drug molecule and properties of the self assemblies in encapsulation along with loci of partitioning. It is also observed that self assemblies of non-ionic molecules allow partitioning of drug molecules in a sequential manner. Experiments on interactions of drug molecules upon release from such assemblies with the target protein have suggested that the binding process is not appreciably different than in that in the absence of self assemblies. The effect of drug delivery vehicles on the thermal and structural stability of target protein (taken as transport protein bovine serum albumin and human serum albumin) have been investigated quantitatively. The results have been correlated with different class of drugs of different nature to understand the role of molecular features in the partitioning process. These studies have significance in understanding the physical chemistry underlying partitioning of a variety of drug molecules into suitable delivery vehicles and permit establishing structure-property-energetics relationships.¹⁻³ Such studies provide general guidelines towards a broader goal of rational drug design.

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Minimalist Peptide Engineering at the Nanoscale for Applications in Healthcare

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Self-assembly of biomolecules to form hierarchical supramolecular ordered structures is emerging as a promising area for fabrication of highly functional smart biomaterials. Peptide based self-assembled structures i.e. molecular hydrogels have gained tremendous interest due to their unique physicochemical properties emergent at nanoscale, which can find important biomedical applications. In our work, we aim to develop the novel biomimetic functional scaffold using self-assembling bioactive peptide sequences for designing an extracellular matrix (ECM) mimic for tissue engineering applications. We used a minimalistic approach which involves the synthesis of short peptide sequences derived from the natural proteins, like, laminin, fibronectin and collagen etc.. We, for the first time, explored the library of structurally related pentapeptides derived from a natural extracellular matrix protein, Laminin, which plays crucial roles in cell adhesion, migration and proliferation. We demonstrated the non-traditional solvent mediated approach to induce supramolecular gelation and access diverse nanostructures. To construct a better mimic of natural ECM, we developed the conjugate gels from collagen and laminin mimetic peptides. The conjugate matrix offers an advantage of incorporating the properties of both structural as well as functional peptide segment of natural ECM. Further, we studied differential interaction of cells with variably modified peptide gels. The studies revealed the necessity of proper hydrophobic-hydrophilic balance of a molecule for preferred bioactivity. Further, to attain diversity within single gelator domain, we employed a simple and unique approach of exploring metal ion interactions to provide a convenient means to access diverse gels from single precursors, with reduced defects and enhanced complexity. Another simpler approach was focused on applying a heat/cool cycle over sonication to induce differential gelation behavior in a single gelator template. These different pathways lead to either kinetically trapped or thermodynamically favoured states giving rise to diverse hydrogels. The gels were found to be thermoreversible and self-healing which induces the injectable behavior in these designer gels. Furthermore, these gels are found to direct the formation of anisotropic rectangular gold nanoparticles within the hydrogel template. The resulting new materials are further modified with specific carbohydrate moieties, such as, cellulose to create peptide-polysaccharide conjugates. We anticipate that our approach of combining peptides and sugars will result in creation of self-assembled nanomaterials which will be capable to foster the chemical and mechanical needs to be a superior surrogate of natural ECM. Ongoing studies are focusing on the futuristic application of these biomolecular gels of variable stiffness towards controlling stem cell differentiation.

Control Drug Delivery for Better Healthcare

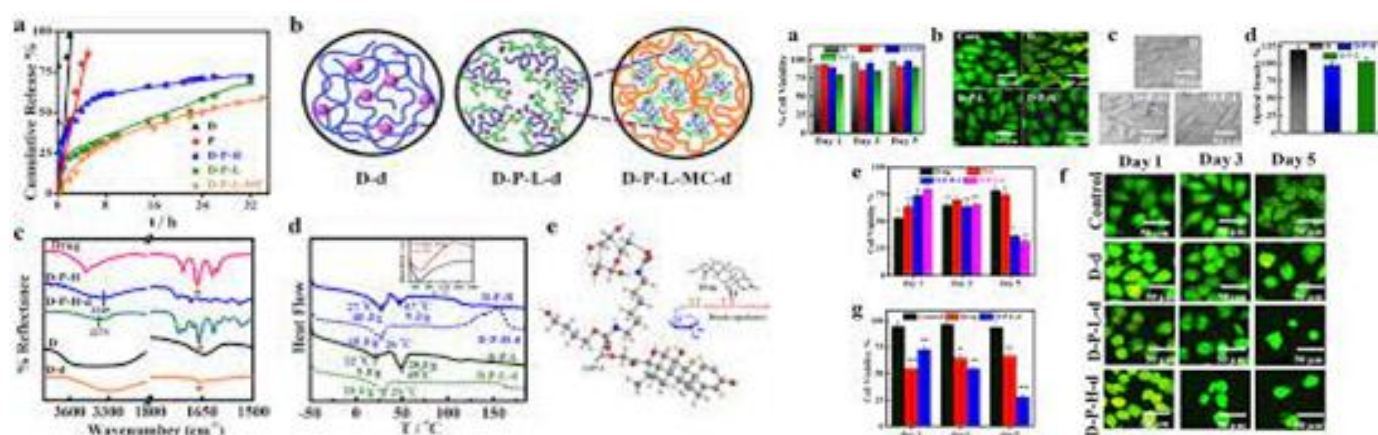
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Variety of molecules has been developed for long term drug release by controlling hydrophilic-hydrophobic balance for effective healthcare. Different generations of molecules are designed through urethane linkages using small spacer to create a large hydrophilic core which is covered with hydrophobic layers of polyurethane through grafting to maintain the hydrophilic hydrophobic balance of the whole superstructure. Drug release becomes sustained from the intricate superstructure following the non-Fickian diffusion process resulting massive cancer cell killing as compared to low killing rate from the pure drug/material arising from its burst release. The superstructure is found to be a good biomaterial and its drug loaded conjugate as carrier is applied to albino mice to treat their tumor, generated through melanoma cell line. Drug embedded superstructure is inoculated in injectable hydrogel and is placed in subcutaneous, below the tumor site, which completely heal the melanoma. No side effect is observed, as opposed to conventional/control system, due to sustained drug release from the superstructure as evident from histopathological studies of sensitive body organs and biochemical parameters. Thus, new design of vehicle heals the melanoma tumor by enhancing the bioavailability of drug and specific interaction without having any side effects as opposed to conventional chemotherapeutic treatment. New design of vehicle will be discussed in details which heal the melanoma and breast tumors by enhancing the bioavailability of drug and specific interaction without having any side effects. Biomaterials for overall healthcare technology will be discussed including bone healing, stent and suture based on shape memory polymers.



Keywords: Polymers, Hydrophilic-hydrophobic balance; Drug delivery; Healthcare.

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Michael Addition Reaction for Achieving Durable Bio-inspired Liquid Wettability

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The nature-inspired wettabilities are with immense potential for various prospective applications including oil/water separation, anti-corrosion, underwater robotics, protein crystallization, drug delivery, open microfluidics, water harvesting etc. In common practice, essential chemistry and appropriate topography that conferred the special liquid wettability were mostly achieved by associating delicate chemistry. Eventually, the synthesized materials suffered from poor durability issue. To develop durable and functional bio-inspired wettability, recently, we have extended 1,4 conjugate addition reaction between amine and acrylates at ambient condition. Further, porous and chemically reactive interfaces were prepared for tailoring various important and functional liquid wettability. Even a strategic association of crosslinker can provide a highly tolerant and hard superhydrophobic coating on a geometrically complex and soft materials. Such simple chemical approach also allowed to reveal important fundamental aspects related to different bio-inspired wettability. Taking advantage of the durable bio-inspired wettability, synthesized nature inspired interfaces were successfully applied to demonstrate some practically relevant out door applications—including oil/water separation, water harvesting etc.

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IL-6

Encountering Emulsion formation at Oil Production and Processing Units (up and down stream) and smarter way of utilizing Emulsion Breaker (Demulsifier) chemistries at various Process Units.

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Crude oil emulsions are observed to form in almost all aspects of oil production and processing: inside oil wells and surface processing facilities and during pipeline transport, crude oil storage and refining. The emulsion has to be treated to remove the dispersed water and associated inorganic salts to meet specifications for transportation and export and to reduce operational issues like corrosion and poisoning of catalysts in different refinery unit operations. The higher energy consumption in transporting crude emulsions also results in an increased carbon footprint for operators. A stable crude oil emulsion is formed when oil and water come into contact and there is sufficient shear and the presence of indigenous surface active materials like asphaltenes, resins, oil wettable solids and other injection chemicals in the recovered crude. Emulsion separation can be a challenge and involves disrupting emulsifying films around water droplets using thermal, chemical and electrical processes. The most common chemical method is addition of demulsifiers or Emulsion Breaker (EB) chemistries to a thermal or electrical process to aid and enhance the separation and removal of water and contaminants.

This talk will give an overview of common treatment processes deployed in oil production and petroleum refining industries to achieve separation of crude oil-water emulsions. The impact of critical process and field parameters such as crude oil characteristics, brine composition, pressure, temperature, solids and other chemical additives on the stability of emulsions and the importance of key criteria that oilfield operators and refiners use to test and screen demulsifiers such as residual water, oil and salt will be discussed. The different classes of chemistries typically used in demulsifier applications and their structure-property relationship will be described. In addition, a few case studies where SUEZ has successfully applied demulsifiers to treat challenging crude emulsions will be discussed to illustrate how a strong understanding of interfacial phenomena can help solve real world problems in the Oil & Gas industry.

Triple-Mode Orthogonal Emission Color Tuning with White Light ON/OFF Switching from a Trimolecular Cocktail in Cationic Micelles for Prospective Anticounterfeitng Applications

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Photoluminescent formulations (single or multi-fluorophore), possessing the unique property of shifting their emission wavelengths in response to different stimuli such as the pH, temperature, ionic strength, solvent polarity, variable excitation wavelengths, etc. are fascinating to explore due to their importance in highly useful areas like white light generation, optical memory systems, bio-imaging probes, encryption/decryption protocols, information display, fluorescent sensors, optical-recording, fluorescent inks, anti-counterfeiting technologies, and even in data storage. White light generation, in particular, is crucial because of its critical importance in current and future generation lighting technology. Therefore finding easy and economical methodologies for the fabrication of such photoluminescent formulations is the need of the hour. I would present our research work related to the development of a simple and eco-friendly aqueous-based three-fluorophore photoluminescent formulation showing emission color tuning in response to different stimuli i.e. the composition of the system, pH, excitation wavelength, and the temperature with the plus point of getting significantly pure white light emission (WLE). The novel system was fabricated from the aqueous mixture of three organic fluorophores, Umbelliferone (**UMB**), Fluorescein (**FLU**), and Rhodamine-B (**RB**). By varying the fluorophore composition in the mixture at pH 12, nearly pure WLE with Commission Internationale d'Eclairage (CIE) 1931 profile of (0.33, 0.33) was obtained at the excitation wavelength of 365 nm, the sustainability of which is ensured by employing the micellar self-assemblies of tetradecyltrimethylammonium bromide (**TTAB**) molecules. Similar WLE was obtained in mildly acidic conditions (pH 6) but at the excitation wavelength of 330 nm. By proper tuning of pH, and the wavelengths of the system to use it as fluorescent ink, we found a remarkable and highly applicable phenomenon observed for the first time i.e., triple-mode orthogonal emission color tuning with white light ON/OFF switching. We validated the vital applicability of this phenomenon in protecting the authenticity of the document with its hard to counterfeit property. Moreover, the emission color of the PL system was explored lucidly for its temperature dependence owing to the thermal responsiveness of **RB** emission, where the PL system proved to be a full-color RGB system.

Fractional additions - Large property changes**Sunil S Bhagwat**

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Surfactants in mixtures often behave markedly differently in terms of functional/performance properties as compared to the individual surfactants. Often, this results in an enhancement in the performance properties, a phenomenon termed as synergism. There are several applications where changing surfactant ratio in the micelle with dilution is exploited for varying properties of the solution including dishwash applications, fabric wash as well etc. The synergism for three surfactant mixtures has been studied - SLS and Triton X100, SLS and CTAAc, Triton X100 and CTAAc. The SLS - Triton X100 mixture was studied for its CMC behaviour using tensiometry and dye solubilisation. It was found to exhibit significant synergism and its CMC behaviour was modelled using the Rubingh one parameter equation. The system also displayed azeotropic behaviour at a specific mole fraction. The CTAAc was synthesized using CTAB and lead acetate. The CTAAc- SLS and CTAAc -Triton X100 mixtures were studied using dye solubilisation and were found to display marked synergism with regards to their CMC. The CMC behaviour of the mixtures required a two parameter equation inspired by phase equilibrium thermodynamics for the SLS -CTAAc system, while for the Triton X100- CTAAc system the conventional one parameter equation was good enough for the fitting

Responsive DNA Nanostructures for Cancer Therapy

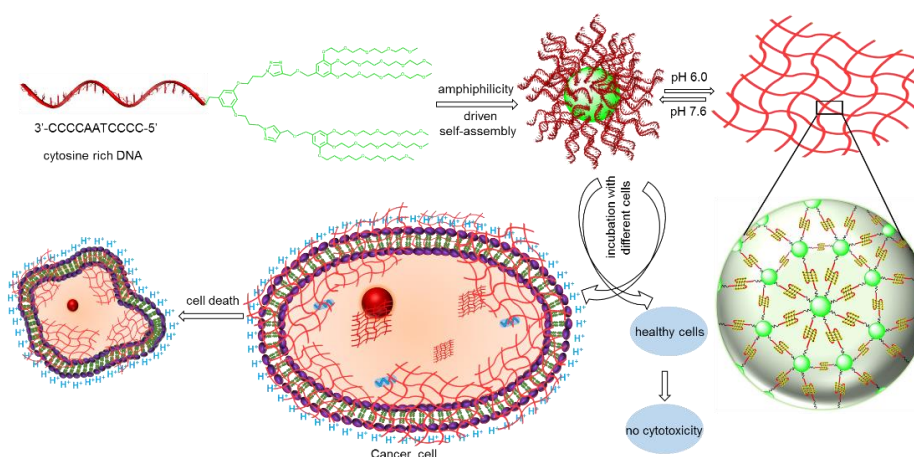
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Improving the effectiveness of the anticancer drugs while minimizing their side effects is a great challenge in cancer research. Recent research efforts in this direction have shown that encapsulating the cell in a gel network can lead to the cell death. Considering the high proton gradient along the cancer cells membrane, we have designed a pH responsive DNA based smart material

which contains C-rich DNA as hydrophilic domain and glycol dendron as a hydrophobic domain, which will self-assemble into micellar nanostructure in basic environment, on acidification cytosine gets protonated and forms inter molecular i-motif, which brings them together and leads to the formation of entangled network. These networks could entrap water molecule which leads to the formation hydrogel. The pH triggered i-motif formation and the fusion of the micelles have been characterized using different spectroscopic and microscopic



Scheme 1: Design of a pH responsive hydrogel for the selective inhibition of cancer growth.

analysis. The hypothesis was examined using three different cell lines, HeLa, A549 and HEK, where HeLa and A549 cell lines are cancer cell line and HEK is healthy cell line. MTT assay analysis reveals that pH responsive hydrogel is highly cytotoxic for the cancer cell lines and biocompatible for the healthy cell lines. Moreover, CLSM analysis on HeLa cell line showed an extra cellular gelation. Our results suggested that pH responsive hydrogel is a good candidate for the selective inhibition of cancer growth (Scheme 1). Details of these results will be presented.

IL-10

Dynamic Modulation of Surface pH of a Catalytic Nanoparticle

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Understanding solid-liquid interfacial chemistry is of fundamental importance in various scientific disciplines ranging from catalysis, energy materials, biosensing and other related (nano)technologies.¹ Notably, many industrial chemical processes rely on solid nanoparticle based catalyst in liquid medium.

At present, attention has been given toward the development of “smart” and “systemic” catalysts which can simultaneously be adaptive and dynamic to obtain nature-like functions, such as time regulation, environmental sensitivity, substrate promiscuity, and modular specificity toward diverse substrates.²⁻⁴ In this direction, we have now developed a CTAB-capped cationic nanoparticles-based catalytic system which can be modulated for its performance by changing the number of phosphate groups (negatively charged group) in self-assembling units (AMP/ADP/ATP). As there is only one phosphate group in AMP, it interacts very loosely with the cationic surface as compared to ATP, having three phosphate groups, thanks to multivalent interaction.⁵ In particular, we have demonstrated that the catalytic preference and activity of the nanoparticle can be directed in a controllable manner towards either hydrazone formation or a proton transfer reaction by changing its interaction from ATP to AMP. Alteration of local surface pH of the GNP due to assembly of these differently charged nucleotides is the key reason for this convertible and tunable catalytic behavior. In addition, catalytic activity and preference of the system can be changed in temporal manner by integrating ATP-hydrolyzing enzyme in the system.

Additionally, differential response behaviour of interfacial pH when pH gets altered in the bulk due to external enzymatic action, for example - nanoparticle surroundings gets acidic by the action of glucose oxidase or basic in presence of urea as a function of time. Simultaneously the effect in catalytic ability of the nanoparticle towards the above-mentioned reactions will also be discussed under changing environment.

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ORAL
PRESENTATIONS

Hydrodynamic and Conformational Characterization of Aqueous Sodium Alginate Solutions with varying Salinity

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Understanding the macromolecular conformation is critical, as the properties and the applications of biomacromolecules depend upon them. One of the basic characteristics of biomacromolecules is their molecular rigidity/flexibility. The molecular rigidity/flexibility of polysaccharides also determines whether the complexation between proteins and polysaccharides results in the formation of coacervates (liquid–liquid phase separation) or complexes (solid–liquid phase separation). Insight into the role of electrostatic interactions on the hydrodynamics and rigidity/flexibility of macromolecular chains in aqueous sodium alginate, an anionic, linear, and water-soluble polysaccharide, was gained through viscometry. Alginate chains are found to shrink in salt-free solutions more rapidly with increasing polymer concentration compared to salt solutions. For salt-free solutions, a reduced polymer concentration of less than 1 suffices to make the alginate coil volume half of that at infinite dilution which becomes invariant when the reduced concentration exceeds 8. In saline media having a salt concentration greater than $0.1 \text{ mol}\cdot\text{L}^{-1}$, the chains become more flexible, caused by the shielding of intra-chain repulsions. The chains effectively reached the unperturbed state when the added salt concentration becomes $\geq 0.5 \text{ mol}\cdot\text{L}^{-1}$. Alginate chains are shown to remain stiff up to about 8-10 monomers within the investigated temperature range. This study explores the possible modification of the individual chain behavior induced by the neighboring chains or by the variation of temperature.



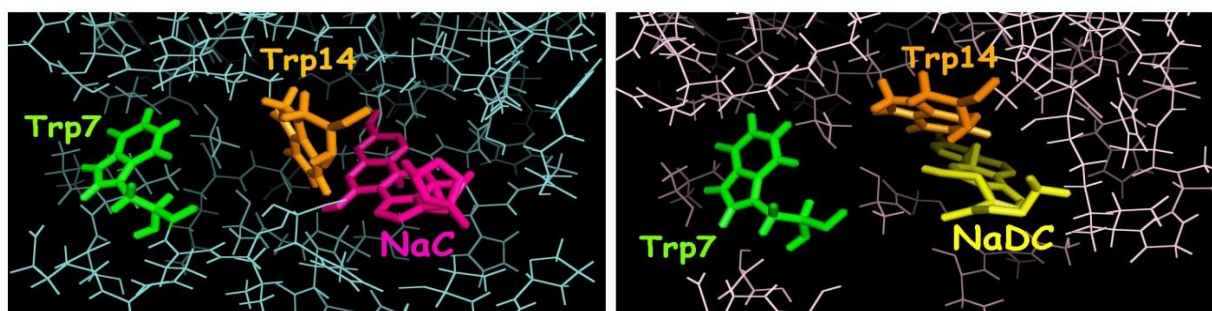
Interaction of the Heme Protein (Myoglobin) with Sodium Salts of Cholic and Deoxycholic acids in Phosphate buffer: A Detail Physicochemical and Molecular Docking Investigation

Arpan Mal, Nitai Patra, Ankur Bikash Pradhan, Satya Priya Moulik and Soumen Ghosh*

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Previous investigation on elaborate study of protein-surfactant interaction has shown that cationic, anionic, gemini surfactants can nicely interact with myoglobin (Mb) than nonionic surfactants. The present study focused on the interaction of one heme protein myoglobin (Mb) with water soluble anionic surfactants such as sodium cholate (NaC) and sodium deoxycholate (NaDC) which acts also as bile salts. The interaction of NaC and NaDC, with myoglobin has been probed by employing different physicochemical and spectroscopic techniques such as tensiometry, UV-vis spectroscopy, fluorometry, time resolved fluorometry, and calorimetry at physiological pH of 7.4 and 298 K. Tensiometric profiles of NaC and NaDC show different nature in presence of myoglobin which is not similar when any charged surfactants have been used. All the three distinct break points observed in presence of heme protein have been supported from tensiometry, UV-vis spectroscopy, fluorometry, time resolved fluorometry and microcalorimetry. The micelle formation of surfactants may alter the conformational change of protein structure causing protein denaturation, and finally, free micelles are formed on further addition of surfactant. Binding between surfactants with the tryptophan moieties present in the heme proteins is described by the help of fluorescence life time measurement. The thermodynamic properties of each successive interaction process have been studied from isothermal titration calorimetry (ITC). The interactive scenario between protein, Mb with surfactants (NaC or NaDC) has also been shown by the light of molecular docking analysis. In this report, the whole study describes a total survey of two anionic surfactants (biles salts) with heme protein interaction at pH=7.4 (phosphate buffer) by employing various techniques.

Keywords: Heme protein, bile salts, molecular docking, various techniques.



Stereo view of the docked conformation of the BS with Mb.

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Micro-Structural investigations on Oppositely Charged mixed Surfactant gels with Potential Dermal Applications

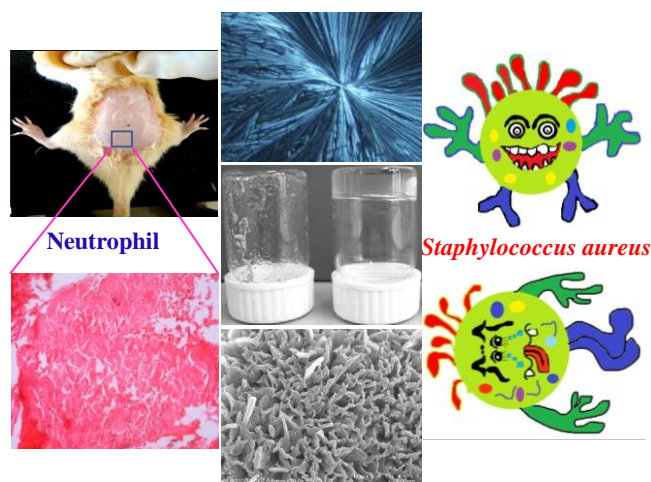
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Dicarboxylic amino acid-based surfactants (*N*-dodecyl derivatives of -aminomalonate, -aspartate, and -glutamate) in combination with hexadecyltrimethylammonium bromide (HTAB) form a variety of aggregates. Composition and concentration-dependent mixtures exhibit liquid crystal, gel, precipitate, and clear isotropic phases.¹ Liquid crystalline patterns, formed by surfactant mixtures, were identified by polarizing optical microscopy.² FE-SEM studies reveal the existence of surface morphologies of different mixed aggregates. Phase transition and associated weight loss were found to depend on the composition where thermotropic behaviours were revealed through combined differential scanning calorimetry and thermogravimetric studies.³ Systems comprising more than 60 mole% HTAB demonstrate shear-thinning behaviour. Gels cause insignificant toxicity to human peripheral lymphocytes and irritation to bare mouse skin; they do not display the symptoms of cutaneous irritation, neutrophilic invasion, and inflammation (erythema, edema, and skin thinning) as evidenced by cumulative irritancy index score.⁴ Gels also exhibit substantial antibacterial effects on *Staphylococcus aureus*, a potent causative agent of skin and soft tissue infections, suggesting its possible application as a vehicle for topical dermatological drug delivery.

Keywords: Hydrogel, liquid crystal, texture, *Staphylococcus aureus*



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OP-4

Transmembrane $\text{Cl}^-/\text{HPO}_4^{2-}$ Antiport Activities of 2-Benzimidazolylthiourea Receptors

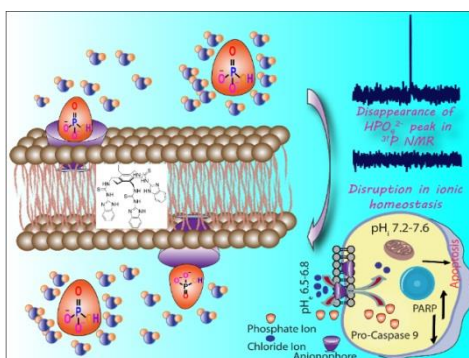
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Transport of anions across the cell membrane is obligatory for regulating various cellular processes in cells. Multifaceted protein machinery facilitates the transport of ions and other charged species across the hydrophobic lipid bilayers.¹ Misregulation of these natural transport systems due to mutation of the transmembrane proteins directly or indirectly regulates various diseases.² The synthetic compounds adept in simulating the cellular functions of the natural protein-machineries are considered as an unconventional strategy to fight against 'channelopathies'. Last few years have seen the widening of the horizons of anion binding receptors for two of the most biologically important anions, sulfate and phosphate with high hydration energies. In view of this, we report the development of 2-benzimidazolylthiourea-based preorganized scaffold displaying good efficacy in phosphate and sulfate transport. The potent tripodal compound shows a higher binding affinity for the oxyanions than the less hydrophilic Cl^- ion and follows the $\text{Cl}^-/\text{HPO}_4^{2-}$ antiport pathways. The alteration of Cl^- and HPO_4^{2-} anion homeostasis in the cancer cells (HeLa) showed induction of apoptotic pathways in the presence of the potent compound, which can be utilized for further medical applications in the future.

Keywords: Channelopathies, $\text{Cl}^-/\text{HPO}_4^{2-}$ Transporter, 2-Benzimidazolylthiourea Derivatives.



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Artificial Hydrolase: Systematic Development and Immobilization on Silica Surface for Enhancement of Activity, Enantio-Selectivity and Reusability

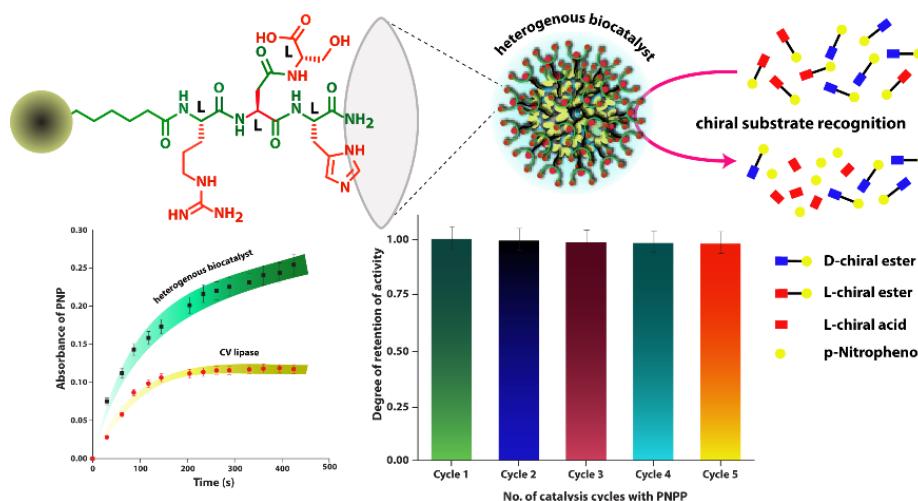
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Biocatalysis is an important area of modern research and is extensively explored by various industries to attain greener methods in various applications. Supramolecular interactions of short peptides have been under the scanner for developing artificial smart materials inspired from natural systems. Peptide-based artificial enzymes have been proved to show various enzyme-like activities.¹ Therefore, immobilization of catalytic peptides on solid surfaces can be an extremely useful breakthrough for development of cost-effective catalytic formulations.² To this end, a catalytic triad, 'Asp(Ser)His', containing peptide amphiphile was immobilized onto silica nanoparticles through covalent bonding method to obtain surface coated catalytic silica nanoparticles. This heterogenous catalytic formulation not only showed enhanced esterase activity than the self-assembled peptide amphiphile in homogenous phase, but also exceeded the activity of natural CV lipase containing 70 units. The catalytic formulation showed incredible stereoselectivity towards chiral esters of an amino acid. The catalyst remained stable at higher temperatures and retained its activity to the fullest after several catalytic cycles.

Keywords: Biocatalysis; Peptide; Heterogenous catalysis; Stereoselectivity; Reusability.



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Smart Microgel-Stabilized Pickering Liquid Crystal-in-Water Emulsions and their Response Towards Amphiphiles

Shikha Aery and Abhijit Dan

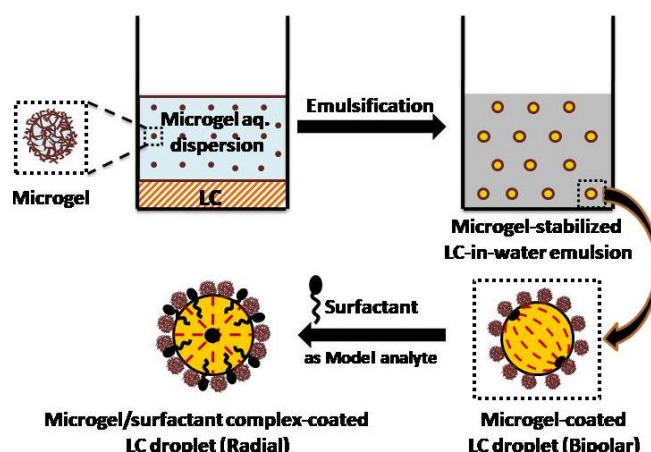
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Liquid Crystal (LC)-in-water emulsions are new generation optical sensors, which consist of micrometer-sized LC droplets dispersed in aqueous media.¹ They are widely used in highly sensitive detection of a range of chemical and biological analytes. In presence of analytes the LC droplets undergo ordering transition, resulting in a change of optical appearance observed under Polarized optical microscope.² But due to various factors such as instability to coalescence, inability of bigger droplets to undergo analyte induced-transition, the bare LC emulsions show poor shelf-life and fail to provide reliable results for quantitative analysis of targeted analytes, thus making them unfavourable for the use in clinical settings.³ Microgels are colloidal particles consisting of chemically crosslinked 3D polymer networks with size typically in range of several micrometers down to nanometers. The poly (N-isopropyl acrylamide) (PNIPAM) microgels are widely used thermoresponsive soft particles, whose size significantly decreases with increase of temperature above $\sim 32\text{ }^{\circ}\text{C}$.⁴ They are known to act as an effective stabilizer (i.e. Pickering emulsifier) for oil-in-water or water-in-oil emulsions. Herein, we report the use of PNIPAM microgels for the stabilization of LC-in-water emulsions. The PNIPAM particles spontaneously and irreversibly adsorbed at LC-water interface, and provided Pickering stabilization to resultant emulsions with remarkably enhanced shelf-life. Despite interfacial microgel coating, the analytes were able to interact with LC droplets and induce observable transition using two possible pathways such as microgel pores and/or interfacial pores present between adsorbed-microgel particles. The coated droplets response was found to be dependent on the charge of the analytes, concentration of microgel and number of LC droplets exposed to analytes. The results show that the PNIPAM-stabilized LC-in-water emulsions overcomes the intrinsic limitations of using bare emulsions in clinical settings and provides a next generation optical sensor that can be used for both reliable quantitative and qualitative detection of targeted analytes.

Keywords: Liquid crystal-in-water emulsions, Microgels, Pickering stabilization, Optical sensors



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Industrial Lecture

Dynamic Light Scattering (DLS) and Electrophoretic Light Scattering (ELS) Technique and Application

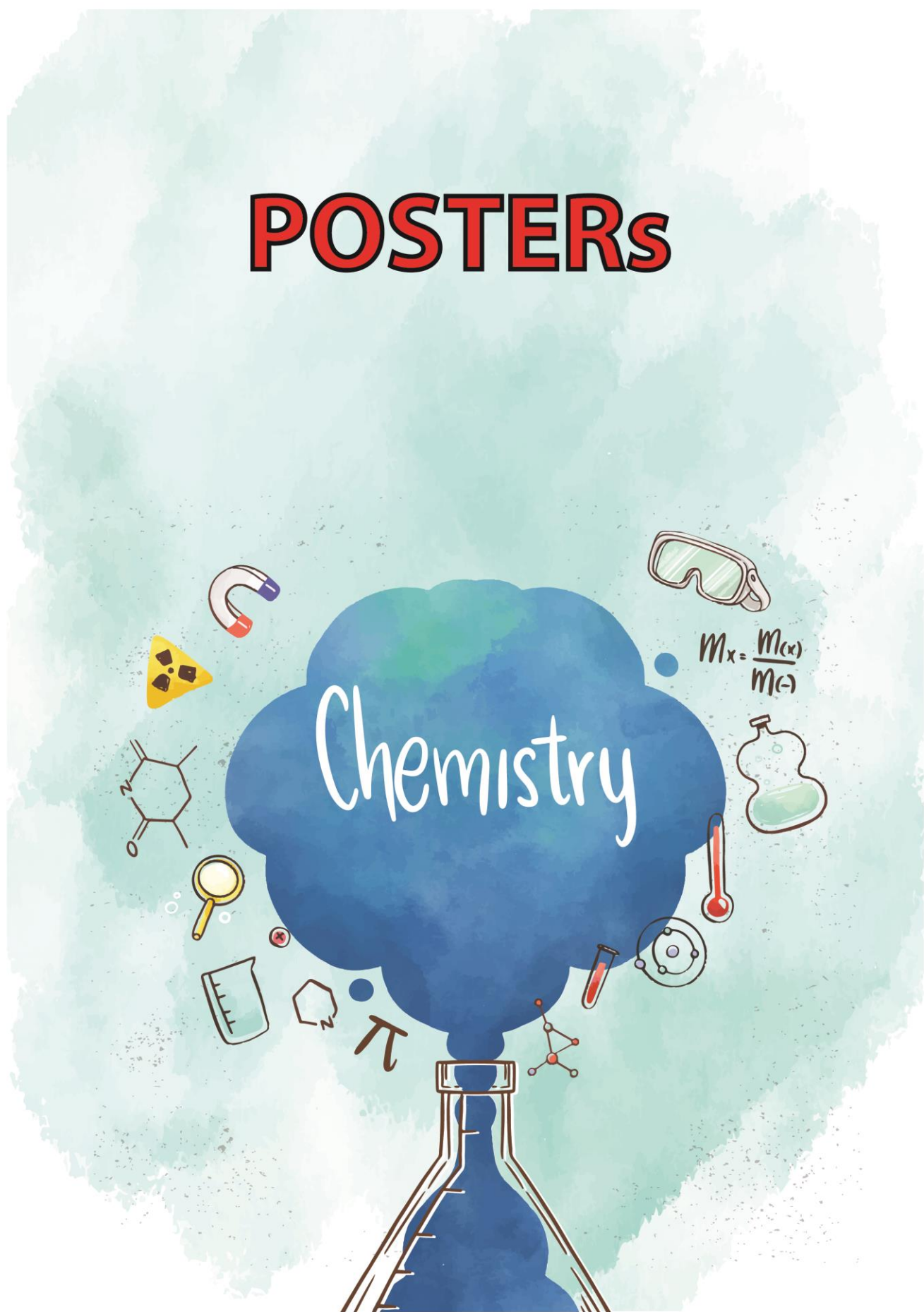
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Nanoparticles have shown immense potential in array of industrial sectors and hence the characterization of their intrinsic properties viz., size, charge and stability are of utmost importance. Light scattering offers a quick, easy and non-invasive technique for these measurements. In this webinar, we will discuss about the basics of these light scattering approaches including DLS and ELS techniques. Besides, glimpses will also be shared about the data interpretation and validity of methods for these techniques and their use in different industrial applications.



POSTERS



P-1

Exploring the Adsorption Efficiency of a Novel Cellulosic Material for Removal of Food Dye from Water

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A cellulosic nanoadsorbent was developed from the fruit coat of Kendu (*Diospyros melanoxylon*), a forest tree, to remove tartrazine (food dye) from the aqueous solution. The nanoadsorbent was synthesized, and its proximate and mineral content were analyzed by AOAC methods. The X-ray diffraction studies established the cellulose I polymorph structure of the bionanomaterial. Fourier Transform Infrared Resonance (FTIR) spectroscopy probing confirmed the presence of the "fingerprint region" in both the virgin Kendu fruit coat and synthesized cellulose nanocrystal. The absence of the lignin and hemicellulose peaks in the FTIR spectrum further supported the formation of the cellulosic nanocrystal. The analysis of morphology of crystal through Transmission electron microscopy envisaged the spectral nature of the crystal with particle size of around 36 nm. The optimal adsorption of tartrazine dye was achieved when the pH and temperature of the solution, adsorbent dosage, initial dye concentration, and stirring speed were 6.0, 323 K, 80 mg/L, 10 mg/L, and 200 rpm, respectively. The fabricated nanocrystals possessed higher adsorption efficiency than the virgin Kendu fruit coats. The nanocrystals could remove more than 95% of the dye, whereas Kendu fruit coat powder could remove around 75% of the dye. The mechanism of adsorption of the dye onto the nanocrystal divulged both polar and nonpolar interactions between the two. The overall study indicated that the Kendu fruit coat could be a cost-effective natural bioresource for the fabrication of a nanoadsorbent to remove the food dye from the aqueous solution.

Key words: Adsorption mechanism; Bioadsorbent fabrication; Cellulosic nanocrystal; Langmuir adsorption model; polar and nonpolar interactions, Tartrazine dye removal.

Cadmium Removal by Adsorption: Enhancement by Surfactant Mediation

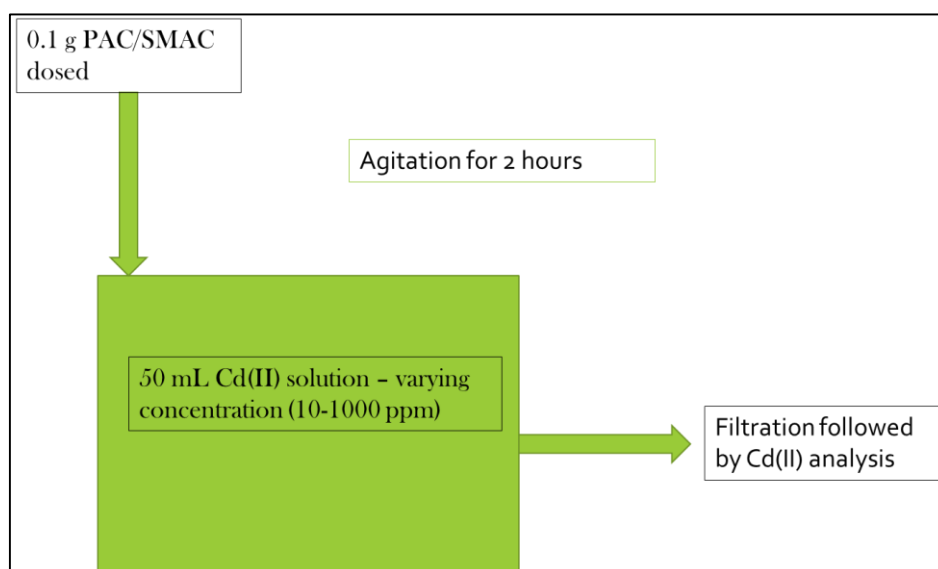
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The presence of heavy metals in water is a matter of great health and environmental concern. This work proposes to tackle the problem of cadmium contamination of water, using adsorption. We have tried to enhance the adsorptive cadmium uptake capacity of activated carbon by modifying its surface with the surfactant - Alpha olefin sulfonate. The effect of contact time and the initial concentration on the adsorption process has been determined. Study of the cadmium uptake by both the unmodified and surfactant modified carbon, with the adsorption data fitted to adsorption isotherms, showed the cadmium uptake capacity of the surfactant modified activated carbon to have enhanced two-fold over the unmodified activated carbon. An attempt is made to elucidate the mechanism for the enhanced cadmium uptake by the surfactant modified activated carbon.



Keywords: Activated Carbon, Alpha Olefin Sulfonate, Cadmium, Surfactant Modified Activated Carbon

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Evolution of Paradoxical Inhibitory Action on Alkaline Phosphatase Bound Liposome in Macromolecular Crowded Environment

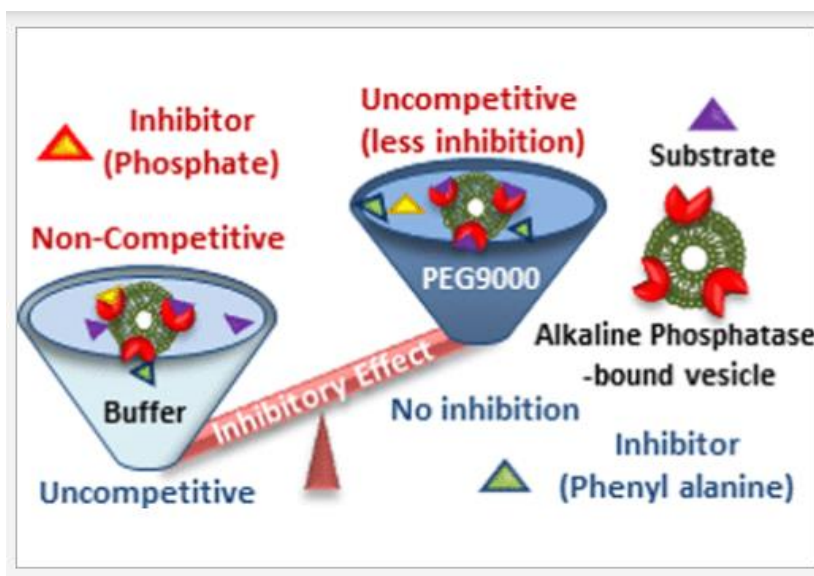
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Nature always been an inspiration for scientists or research scholars in order to mimic, understand the efficient systems prevailing in biological systems like in cellular media. Though it's a very well-known fact that the cytoplasm of a cell is extremely crowded but till today we are not able to completely understand it.^[1] People have studied enzymes in these crowded media and also under high pressure to gain a better understanding of their functioning in aquatic diaspora.^[2] But liposomes under these media are hardly studied which can provide us better comprehension of cellular media.

Cell consists of phospholipid bilayers which play a crucial role in transporting many species in and outside of the cell. Also, a lot of enzymes are membrane bound like Alkaline phosphatase (AP).^[4] Vesicle bound enzyme or Liposomes in macromolecular crowded media presents a model in order to understand the functioning of enzyme inside the cell. Herein, we have used the AP bound vesicles considered as soft particles and microbead tagged enzyme (hard particles) in presence of different crowding agents like PEG 9000, PEG 4000 etc. Also, we have investigated the inhibitory effects of different inhibitors of Alkaline phosphatase on liposome and on bead tagged enzyme in crowded media. To our surprise, the inhibition nature of inhibitors found to be entirely different for liposomes in crowded media. Also, the soft and deformable nature of AP vesicles or liposomes helps them to perform better catalytically in comparison to hard particles or AP tagged beads. This somehow provides us the clearer picture about how membrane bound enzymes are crucial in order to function inside the cell. And how the interface of a membrane bound enzyme and macromolecular crowding can modulate the inhibitory action of inhibitors.^[5]

Keywords: Macromolecular crowding, AP liposomes, Alkaline phosphatase.



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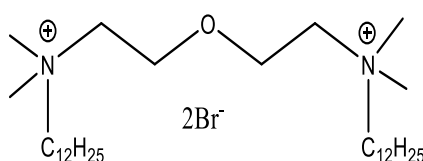
Studies of the Interaction of Gelatin with Gemini Surfactants Having Diethyl Ether Spacers

Anandita Mitra and Pramila K. Misra*

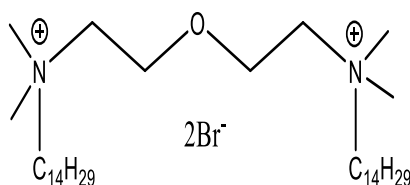
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The interactions and aggregation properties of three cationic Gemini surfactants containing diethyl ether spacer groups with varying carbon chain length ($n = 12, 14$ and 16) and gelatin mixed assemblies in water were investigated using UV-Vis, Fluorescence and Lifetime Spectrometry methods. The interactions with gelatin were analysed with the decrease in Critical micellar concentration (CMC) with the increase in gelatin percentage from 0.1% to 0.4%, for example the CMC of Gemini Z ($n = 16$) with 0.1% gelatin is $9 \times 10^{-5} \text{M}$ whereas in 0.4% gelatin is $6 \times 10^{-5} \text{M}$. For intrinsic fluorescence and anisotropy measurements the graph increased with the increase in surfactant concentration up to a certain maximum value and after that it decreased and became constant with further increase in surfactant concentration. The maximum value is understood to be the point of micellization (CMC) between surfactants and protein. For lifetime of tyrosine, lifetime increased up to the CMC value (as obtained from Intrinsic fluorescence and anisotropy maximum point) and then remain constant with further increase in surfactant concentration. The maximum rigidity of the mixed system was also very much significant from the lifetime data. The polarity parameters of pyrene also added more data to the formation of micelles at higher concentration of surfactant-gelatin mixed systems. The decrease in aggregation no. with increase in gelatin concentration put light on the better compatibility of the surfactants with the environment.

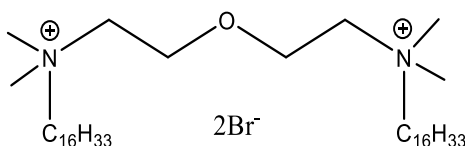
Structures of Gemini Surfactants:



1,4-bis(dodecyl-N,N-dimethylammonium bromide)diethylether (**Gemini-X**)



1,4-bis(tetradecyl-N,N-dimethylammonium bromide)diethylether (**Gemini-Y**)



1,4-bis(hexadecyl-N,N-dimethylammonium bromide)diethylether (**Gemini-Z**)

Dually Reactive Multilayer Coatings Enable Independent Functionalization of Underwater Superoleophobicity and Oil Adhesion

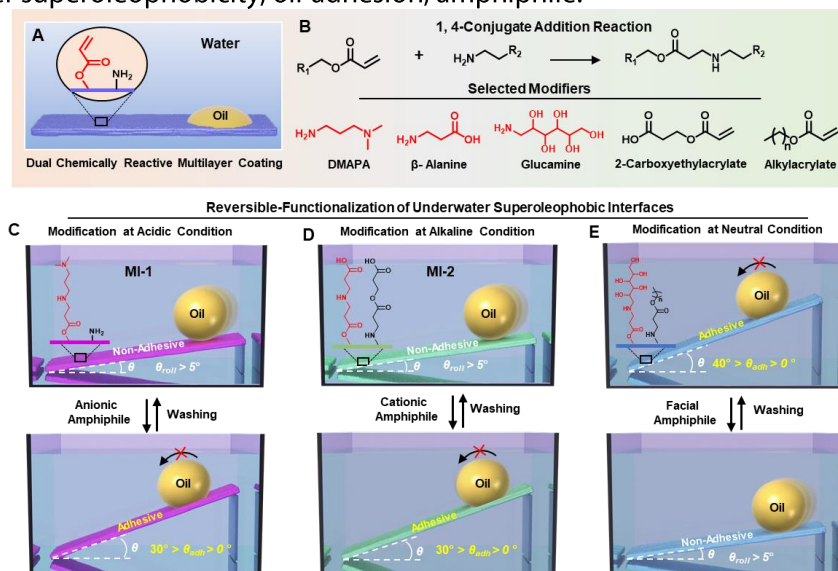
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Fish-scale inspired underwater non-adhesive superoleophobicity is commonly and artificially constructed by creating hierarchical surface topography on water-compatible materials, including polymeric hydrogels, metal oxides, electrostatic multilayers, etc.¹⁻² While such conventional principle of developing underwater extremely oil-repellent interface have been widely exploited in various prospective applications, a fundamentally distinct design of chemically reactive underwater non-adhesive superoleophobic coating with the ability for associating tailored and responsive underwater oil-adhesion independently would likely to extend the horizons of its potential. Here, we design a dually reactive multilayer coating, whose underwater superoleophobicity and oil adhesion can be independently tuned through the orthogonal functionalization of two types of reactive moieties at ambient conditions. Moreover, the cooperative assembly of amphiphiles on the modified underwater superoleophobic coating gives rise to a reversibly switchable oil adhesion while retaining the extreme oil-repellency (advancing oil contact angle $> 165^\circ$). The reversible change in the oil adhesion of the underwater superoleophobic coatings depends on the interplay between the molecular structure and concentration of the amphiphiles and the pH of the aqueous solution. Building on these findings, we developed superoleophobic sensors that enable the real-time identification of (1) the charge of the head group of synthetic ionic surfactants and (2) the concentration of bile acids without complex equipment and procedures. The precise change in oil-adhesion due to adsorption of certain amphiphiles at a particular condition on the underwater oleophobic interfaces was unprecedentedly extended to demonstrate a naked eye, absolutely equipment-free and real-time identification of the physiologically important amphiphiles and metabolites.³

Keywords: underwater superoleophobicity; oil-adhesion; amphiphile.



Scheme. (A-B) Scheme showing dually reactive multilayer coatings (A) and 1,4-conjugate addition reaction (B). (C-E) Schematic illustration of reversible functionalization of underwater superoleophobic interfaces with amphiphiles at specific pH.

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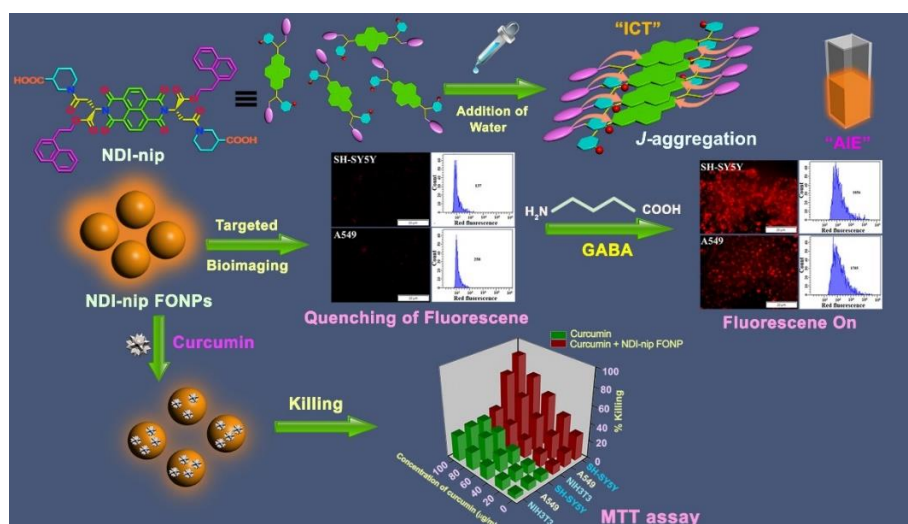
Nipecotic Acid Tethered Naphthalene Diimide based Orange Emitting Organic Nanoparticles as Targeted Delivery Vehicle and Diagnostic Probe towards GABA_A Receptor Enriched Cancer Cells

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Over the past few decades luminescent nanoparticles having aggregation-induced emission (AIE) property drawn enormous attention in across the scientific disciplines primarily as a sensing and imaging tool because of its synthetic ease, cost-effectiveness, high sensitivity and operational simplicity.¹⁻⁴ This present article demonstrates target specific cellular imaging of GABA (γ -aminobutyric acid) receptor (GABA_AR) enriched cells (SH-SY5Y and A549) with therapeutic efficacy by naphthalene diimide (NDI) derived fluorescent organic nanoparticles (FONPs). Self-assembly driven formation of spherical organic particles by nipecotic acid tethered L-aspartic acid appended NDI derivative (**NDI-nip**) took place in DMSO-water through J-type aggregation. **NDI-nip** having naphthyl residue and nipecotic acid unit at both terminals exhibited AIE at and above 60% water content in DMSO due to excimer formation at $\lambda_{em} = 579$ nm. The orange emitting **NDI-nip** FONPs (1:99 v/v DMSO-water) having excellent cell-viability and high photostability were used for selective bioimaging and killing of GABA_AR overexpressed cancer cells through target specific delivery of anticancer drug, curcumin. Fluorescence intensity of **NDI-nip** FONPs got quenched in GABA_AR enriched neuroblastoma cell (SH-SY5Y) and cancerous cell (A549). Notably, in presence of GABA, the **NDI-nip** FONPs exhibited its native fluorescence within the same cell lines. Importantly, no such quenching and regaining of **NDI-nip** FONPs emission in presence of GABA was noted in case of noncancerous cell, NIH3T3. The killing efficiency of curcumin loaded **NDI-nip** FONPs ([curcumin] = 100 μ M and [**NDI-nip** FONPs] = 50 μ M) was significantly higher in case of SH-SY5Y (88 \pm 3%) and A549 (72 \pm 2%) than that in NIH3T3 (37 \pm 2). The presence of nipecotic acid moiety facilitated the selective cellular internalization of **NDI-nip** FONPs into GABA_AR overexpressing cells. Hence, this orange emitting **NDI-nip** FONPs may be exploited as targeted diagnostic probe as well as drug delivery vehicle for GABA_AR enriched cancer cells.

Keywords: Aggregation-induced emission, Naphthalene diimide, GABA_A receptor, Curcumin delivery



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P-7

Removal of Polyoxyethylated Nonyl Phenol from Aqueous Solution by Modified Hydroxyapatite

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The adsorption characteristics of polyoxyethylated nonyl phenols, NP-10, NP-15 and NP-20 surfactants with 10, 15 and 20 oxyethylene units, respectively as the hydrophilic moiety and nonyl unit as the hydrophobic chain is reported in the present study. The greater hydrophobicity resulting in lowering of CMC of NP-10 in comparison to NP-20 was revealed by the surface tension measurement. The adsorption of the surfactants was, however, achieved only after the modification of the hydroxyapatite (HAp) surface by sodium dodecylsulphate (SDS). Thus, SDS plays an important role to bind to HAp through the hydrophobic interaction. Different characterization tools like UV-visible, DLS, and Zeta potential analyses were carried out to investigate the mechanism of adsorption. The increase in the adsorption values with the increase in the concentration was attributed to the hydrophobic association between the nonyl group with dodecyl chain initially (favourable adsorption). The monolayer surface coverage of nonionic surfactant over the modified HAp interface was evidenced from the adsorption isotherm data. The maximum percentage removal of NP-10 and NP-20 was found to be 95% and 77%, respectively under the optimal conditions. The higher percentage removal of NP-10 was attributed to its smaller size in comparison to NP-20.

Conducting Polymer Supported Cerium Oxide Nanoparticle: Enhanced Photocatalytic Activity for Dye Degradation

Boby Samai

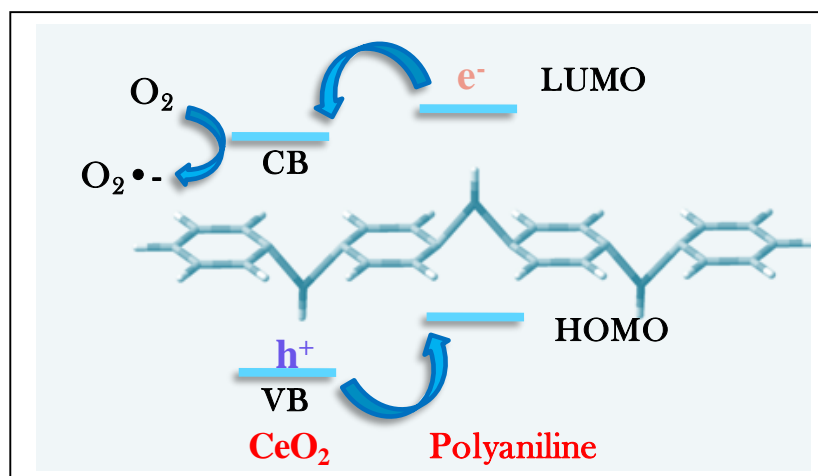
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Photocatalysts are an important milestone for harvesting chemical energy from light energy in the era of massive energy consumption. Cerium oxide nanoparticle (CeONP), having wide application from catalysis to biomedical field, has drawback as photocatalyst due to its large band gap. Herein, a conducting polymer, polyaniline (PANI) has been chosen as active catalyst support to upgrade photocatalytic activity of CeONP. In this article firstly spherical shaped CeONP was prepared by hydrothermal method. Later, PANI was decorated on CeONP surface via in-situ oxidative polymerization of aniline monomer. The as synthesized PANI/CeONP nanocomposite shows remarkably enhanced photocatalytic efficiency in comparison to CeONP or PANI in the degradation of a model organic pollutant Rhodamine B (RhB) in waste water under UV light irradiation. The enhanced photocatalytic mechanism is attributed to the synergistic effect between PANI and CeONP, which reduces recombination rate of photoinduced electron hole pair.

Keywords: Cerium oxide, photocatalyst, polyaniline.



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Metallocatanionic Vesicles Mediated Photodynamic Therapy

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Metallosurfactant (MS) aggregates have grasped great attention from researchers worldwide due to the dual properties of both metals and surfactants. On complexing surfactants with metal ions, depression in the CMC is usually observed compared to those of the parent innocent surfactants^{1,2}. Catanionic vesicles are synthesized by mixing cationic and anionic surfactants into a non-stoichiometric ratio which leads to spontaneous vesicle formations. These vesicles can control the size, surface charge by varying the cationic/anionic ratio. Photodynamic therapy (PDT) is a combination of photosensitive drugs, light and molecular oxygen^{3,4}. We have formulated metallocatanionic vesicles (MCVs) by using Cu and Fe-based cationic MS in PBS of 7.4 pH. In this approach, two of the fractions, one each from a cationic rich and anionic rich side, were selected to encapsulate anionic photosensitizer (PS). These studies reveal that the MCVs have dual functionality *i.e.* encapsulate PSs and even show antibacterial properties against *S. Aureus*, *E. Coli*. MCV help in enhancing the singlet oxygen yield of PS. We have applied these PS-loaded MCV showed biocompatible nature in dark and high phototoxicity against U-251 cancer cell lines. Caspase assay confirmed the apoptotic pathway of cell killing. This work provides a new metal hybrid smart biocompatible material that possesses dual functionality and is prepared by an easy, fast, and feasible procedure which resulted in enhanced PDT against a drug-resistant bacterium and cancer cell lines.

Keywords: Metallosurfactants, metallocatanionic vesicles, singlet oxygen (¹O₂), phototoxicity.

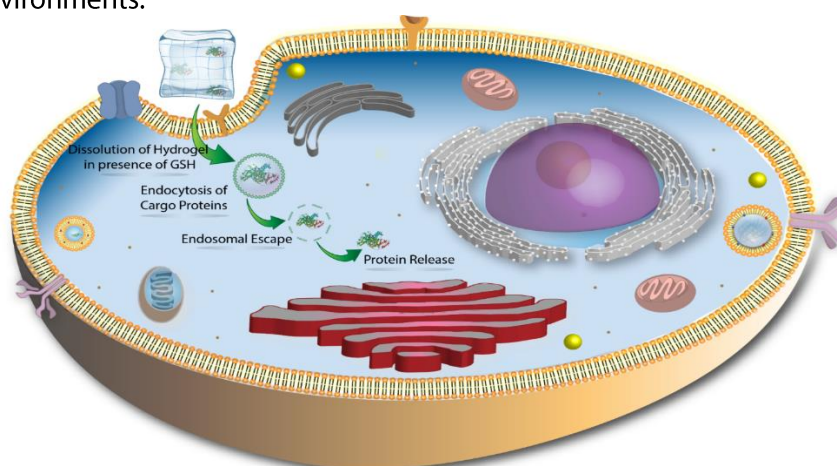
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Protection and Glutathione Responsive Delivery of Proteins by an Ultrashort Peptide Hydrogel

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Protein and peptide-based therapeutics offer the ability to treat diseases such as protein deficiency or mutations, cancer, microbial infections, autoimmune disorders, psoriasis, and diabetes, to name a few.¹ A plethora of carriers for intracellular delivery of proteins and peptides have been charted in the last decade that includes dendrimers, metal nanoparticles, silica nanostructures, protein-based vehicles, lipid-based systems, metal-organic frameworks, vesicles, nanotubes, polymers, virus like particles etc.¹ Based on the previous literature on the same we must conclude that to confront the common shortfall of available delivery vehicles remains in losing activity of the cargo proteins during covalent modification, herein, the supramolecular hydrogel is an attractive alternative. Several peptide-based hydrogels are reported with the ability of cellular protein delivery. However, it is essential to comprehend that protein delivery with hydrogel is technically limited to topical applications unless the hydrogel is injectable/thixotropic in nature. The cargo loaded hydrogel can be injected at the site of treatments. Additionally, the hydrogel must be sensitive to the extracellular environment or to a biomolecule present to release the cargo. In this context, we have recently reported an ultrashort peptide hydrogelator with the ability to form a gel in water that remains insoluble in water and HBS (human blood serum).² However, the **PyKC** hydrogel is responsive to GSH. Additionally, we have shown the very tightly knitted network of the **PyKC** hydrogel is capable of encapsulate and protect proteins from external denaturing effects for a long time without any significant loss of protein activity. Considering the shortcomings of the hydrogel-based protein delivery systems, we envisioned that **PyKC** hydrogel could be a potential candidate for efficient protein delivery. Another essential criterion for the success of such delivery vehicles is that the hydrogel should adhere to the tissue. To resolve this issue, we have prepared another short peptide (**PyKRGD**) containing a known cell adhesive unit, RGD. A composite hydrogel was formulated combining two different short peptides **PyKC** and **PyKRGD** which successively deliver more than 50% of loaded proteins at cellular environments.



Schematic presentation of the plan.

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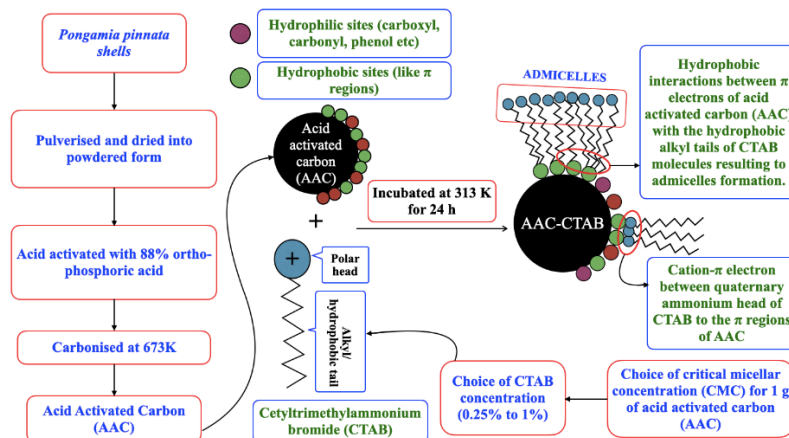
Cationic Surfactant Treatment of Acid Activated Carbon to Augment its Role as an Adsorbent

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Activated carbon is primarily preferred for wastewater treatment and remediation due to its extended surface area, porous structure, high adsorptive capacity and high degree of surface reactivity.¹ For economic scalability, cheap carbonaceous precursors such as lignocellulosic waste materials are preferred for its synthesis. For our study, *Pongamia pinnata* shells were selected as a potent precursor for acid activation followed by thermal carbonisation to prepare low cost acid activated carbon. Acid treatment develops cross-links, leading to a rigid porous matrix and also oxidises the surface, thus rendering it with acidic functional groups. High temperature carbonisation further promotes porous morphology with volatile pore matrices attributing to enhanced surface porosity.² However, activated carbon surface has various hydrophobic regions which makes them less susceptible and dispersive in aqueous medium and thus this affects its uptake capabilities. Surfactants enhance the wettability and reduce the surface tension of activated carbon in order to enhance its performance in aqueous phase and thus they promote the uptake of wide array of organic pollutants like that of phenolics, oil and anionic dyes species.³ Cetyltrimethylammonium bromide (CTAB) is one such positively charged quaternary ammonium surfactant with 16-carbon long alkyl chain and an ammonium head with three methyl groups attached. Being a quaternary ammonium salt, it has large alkyl group which provides CTAB with thermal stability and thus makes it feasible for higher temperatures.⁴ The process underlying the surfactant modification at the solid-aqueous interface is via discrete surface aggregates and not merely the formation of monolayer or bilayer. These surface aggregates formed at certain surfactant concentrations are known as 'admicelles'. Admicelles are usually assembled at surfactant concentrations slightly lesser than the critical micelle concentration (CMC) which is opposite to micelle formation.⁵

Keywords: Cetyltrimethylammonium bromide; Acid activated carbon; Adsorbent.



Graphical abstract presenting the complexation of CTAB over acid activated carbon

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Highly Efficient Purely Organic Triplet Harvesting AIE Photosensitizer for Image-Guided Photodynamic Therapy

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Triplet harvesting image-guided photodynamic therapy (PDT) has been acknowledged as one of the most representative strategies for cancer and other diseases, owing to its precision, non-invasiveness and improved imaging. Unlike, conventional fluorescence molecules with lower sensitivity and hinder high-resolution imaging with cytotoxic heavy metal ion containing metal complexes based photosensitizer for PDT study, here, we formulate purely organic triplet harvesting photosensitizer (PS) BTMCZ, BTMPTZ and BTMPXZ exhibiting thermally activated delayed fluorescence (TADF) and room temperature phosphorescence (RTP) with aggregation induced emission (AIE) characteristics. Remarkably, integrated PSs could generate reactive oxygen species (ROS), singlet oxygen ($^1\text{O}_2$) under white-light irradiation to kill the cancer cells efficiently. In addition, the molecules are self-assemble into nanoparticles/ nano-ribbons and accumulate homogeneously in the cancer cells thereby a high-resolution imaging was recorded. This novel photosensitizer could be a good candidate for cancer treatment in clinical practice.

Keywords: Aggregation Induced Emission; Delayed Fluorescence; Phosphorescence; Photodynamic Therapy.

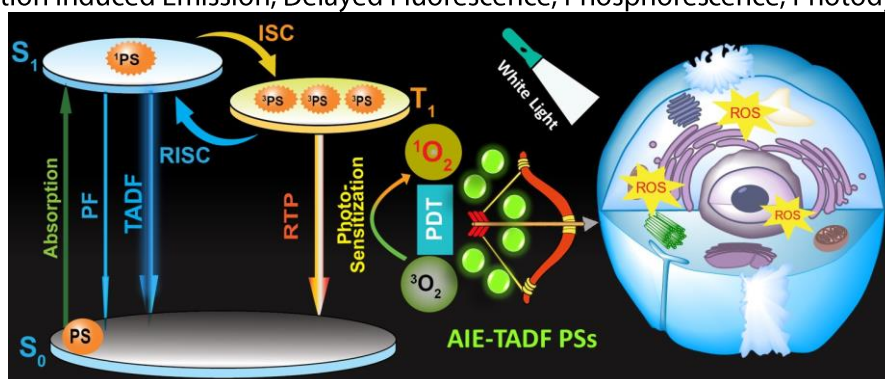


Figure 1: Illustration of TADF and RTP mechanism by Jablonski diagram and representation of reactive oxygen species (ROS) generation for PDT activity in cancer cell.

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Magnetic and Fluorescent Colloidal Nano-Formulations of Hemp Oil

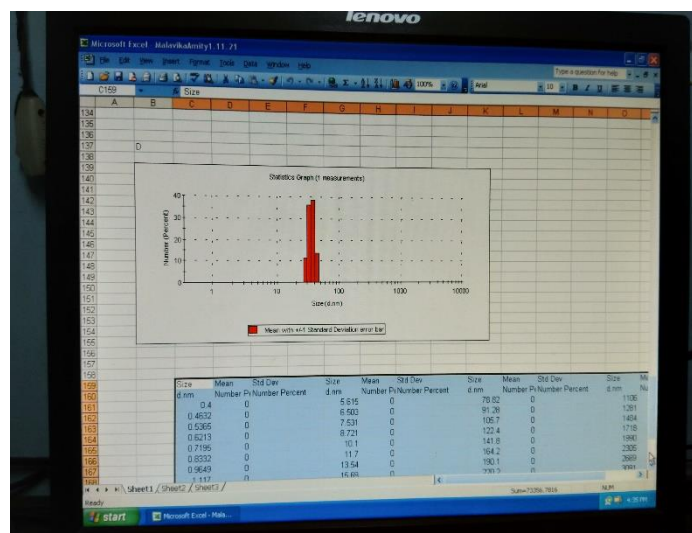
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In this work, we have developed two distinct colloidal nano-formulations of hemp oil one is magnetic nano-particles using hemp as the stabilizer and the second one is carbon quantum dots for fluorescence and study the diffusion of the various drugs in the biological system. Our previous published work showed promising results, where we used magnetic nano-particles coated with oleate and linoleate bilayer as shell. The host-guest type of system was used to design sustain release of doxorubicin (DOX) in a controlled manner [1]. The present work idea is slightly resembling to our previous work but instead of using synthetic compound like oleate and linoleate, we coated our host-system with more biocompatible material like Hemp oil. Hemp oil is mixture of both oleic and linoleic acid and also other fatty acids. Few research has showed the role of Hemp oil against inflammation and possess anti-cancer activity. The colloidal stability of the nano-particles is due to the formation of the bilayer composed of naturally present oleic and linoleic acid moieties in the Hemp oil. The Hemp oil is a natural material obtained from the cannabis plant [2]. The medicinal property of the plant and its extract went unchecked. We even aim to show the various medicinal effects [3] and how it can be used in cancer palliative care to treat pain. Human body has its own endocannabinoid system and natural receptors. The receptors are G-coupled protein receptor namely CB1 and CB2. Using bodies own natural receptors we aim to demonstrate the various benefits of Hemp oil.

Keywords: Magnetic nano-particles; carbon quantum dots; Hemp oil.



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Silver Nanoparticles embedded on *in-vitro* biomineralized Vaterite: A highly efficient catalyst with enhanced catalytic activity towards 4-Nitrophenol reduction

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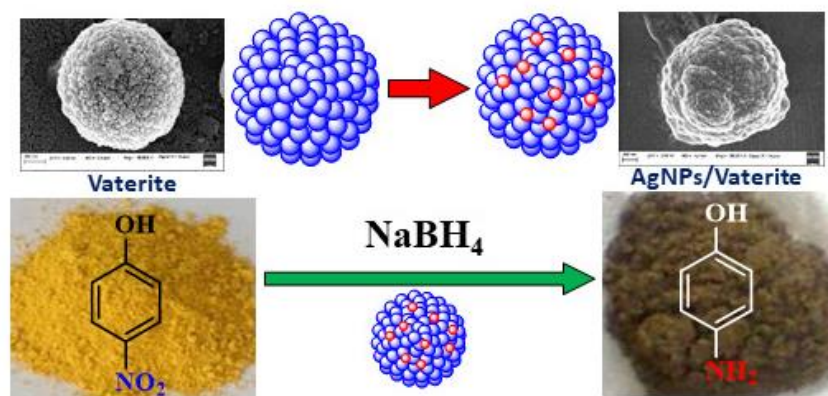
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In vitro biomineralized vaterite with spherical morphology and porous surface texture was utilized as inert solid support for silver nanoparticles to form a composite material that was subjected as a catalyst for the reduction of 4-Nitrophenol. The methods assigned were eco-friendly and one of the highlights was the very even and dense distribution of the silver nanoparticles with no evident signs of agglomeration. The majority of the silver nanoparticles embedded were of ultrafine size and this can be attributed to the porous surface texture of vaterite. The composite catalyst showed excellent catalytic activity and remained unaltered for at least five consecutive cycles. Additionally, to justify its versatility, the effectiveness of the catalyst was studied towards the reduction of 4-Nitrophenol in water from natural sources. Hence, this efficiently designed composite material can be used as a potential catalyst for polluted and wastewater treatment.

Keywords: Biomineralized Vaterite; silver nanoparticles; composite material; heterogeneous catalysis



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Aggregation Induced Emission Enhancement and Selective Detection of Picric Acid in Aqueous Medium

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Picric acid (PA) is a menacing environmental pollutant on account of its high solubility in water. Extensive usage of picric acid as a handy chemical and go-to explosive in pharmaceutical and chemical industries has been posing alarming threats to the environment and public health. The detection of PA in aqueous medium and vapor state is extremely important for military and civilian safety. Here, we report the synthesis of water soluble 1, 8-naphthalimide (ANDI) and multimodal sensing applications of aggregated materials for nitro explosives such as picric acid (PA) in aqueous, solid surface and vapor phase. The ANDI aggregates demonstrated substantial selectivity and ultrasensitive detection of PA with exceptional quenching constant $7.23 \times 10^6 \text{ M}^{-1}$ and limit of detection 149 ppb. The quenching takes place due to ground state charge transfer complex formation between PA and ANDI. Equilibrium simulation and the potential of mean force calculations reveal that the ANDI self-assembly is stabilized by extensive π - π interactions and the primary driving force behind the recognition of PA by the assembly is van der Waals interactions. ANDI aggregates would be potential materials for the construction of low cost and light weight nitroaromatic explosive sensors for future application.

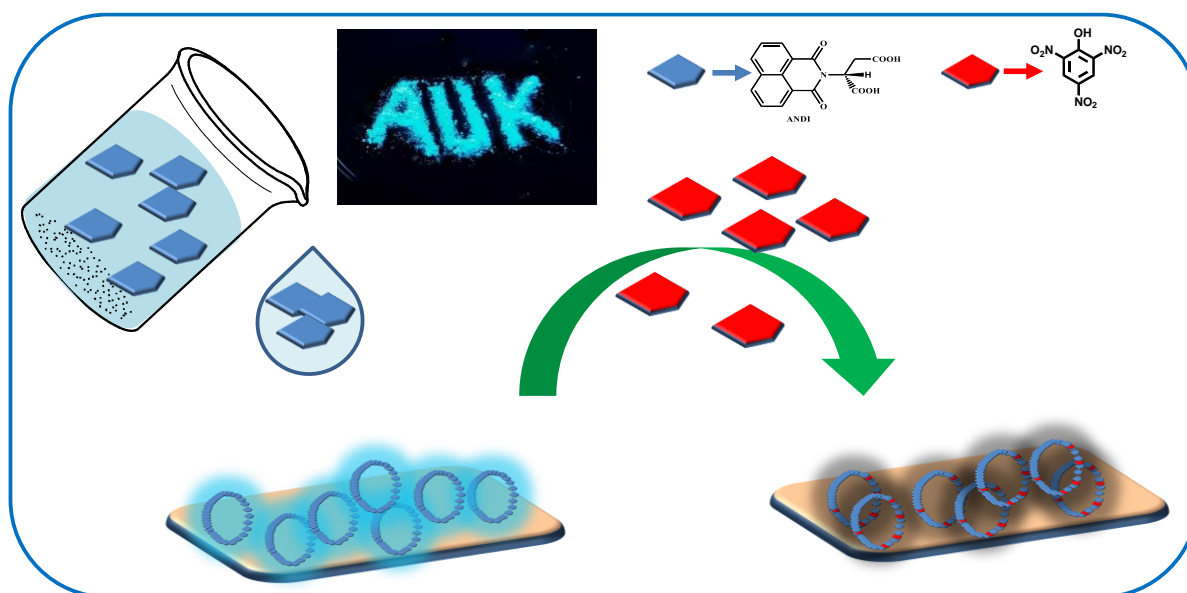


Figure: Aggregation Induced Emission Enhancement in solid state under UV light and its selective detection of Picric Acid (PA) by intercalating PA within the spherical aggregates.

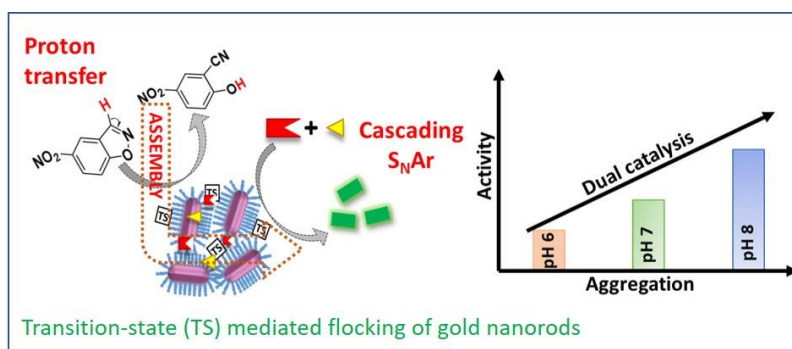
Interconnectivity Between Surface Reactivity and Self-Assembly of Kemp Elimination Catalyzing Nanorods

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Understanding and exploring dynamic behavior of catalysts during catalytic processes is a topic of interdisciplinary interests for both fundamental and applied research. In natural systems, multiple biocatalysts/enzymes form supramolecular assemblies and complexes, like- purinosome (formed during purine starvation), metabolon (sequentially formed enzyme complex during metabolic pathways) etc.¹ While these examples are scarce in synthetically designed catalytic system and mostly for amphiphilic or nanoparticle system by using external trigger which act as a supramolecular template of the building blocks.² Herein, for understanding enhanced diffusion and dynamic interactions between catalysts during assembly formation and catalytic processes, we have designed a synthetic nanocatalytic unit forming functional self-assembly where catalytic process plays the central part. Here, cetyltrimethylammonium bromide (CTAB)-functionalized gold nanorods (GNR) catalyzed Kemp Elimination (KE) reaction (a commonly used model to understand mechanistic intricacies in biotransformation)³ resulted in transition state mediated enhanced flocking behavior of nanorods during the catalytic conversion period to form larger sized assembly. In fact, we have found the assembly rate is correlated with the catalytic activity of the nanoparticle surface. Also, enhancement in diffusion of nanorods during catalytic conversion validated the same. In addition, we have also observed that the hydrophobic cavities formed during flocking of gold nanorods can be utilized for trapping and catalyzing reactions between hydrophobic substrates which otherwise does not occur in aqueous media. Overall, we have demonstrated a catalytic phenomenon that can lead to cascading of other reactions, absolutely unrelated to the original catalytic mechanism.⁴ This finding demonstrates that the fundamental fact of catalyst assembly can be modulated by altering its surface reactivity and this behavior can potentially lead to multiple other events indicating possible emergence of more life-like complex chemical systems.

Keywords: Self-assembly; Surface reactivity; Enhanced diffusion; nanorods.



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Process of Incorporation of Additives using Surfactants to Develop Functional Viscose Fibres

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Viscose fibres are used in making apparels due to their superior properties such as good absorbency, high softness, good dyeability and better drapability. The possibility of using them in functional textiles and technical applications is also immense if the fibres can be engineered as required. This has given rise to increased R&D efforts to develop functional viscose fibres. A feasible way to impart functionality in viscose fibre is through incorporation of functional additives. Incorporation of these additives into the polymer solution prior to spinning not only results in longer lasting effects but also is a greener process. However, there are challenges in making such fibres on an industrial scale. These relate to how the additives interact with the different mediums used in preparation of Viscose fibres. Though few studies are available to provide some insights on this, a deeper understanding was sought to be obtained through this work. In this article, we present a brief understanding of the phenomenon, methods, and process of incorporation of additives in the Viscose process. The evaluations carried out covers effect of 1. Mechanical treatments like ball milling & ultrasonication to reduce the particle size of the additives with optimisation of the process conditions for uniform dispersion and 2. Effect of surfactants to impart better stability to the dispersions. Fundamental understanding obtained through the study is that as the additives are dispersed in water, an interface is created which is hindered by the diffusion of the surfactants to the interface. Adsorption of the surfactants at the surface of the material keep the particles well separated and avoid agglomeration by energy barriers due to electrostatic or steric repulsions. Adsorption of the surfactant depends on the chemical nature and surface charge properties of the additive, and the surfactant used. Characterisation tools for the dispersion studies included particle size and distribution measurement and surface charge measurement. To get good insights, two surfactants of different ionic nature were used to stabilise two different additives i.e. a carbon black based organic pigment and an inorganic metal oxide in the study.

To demonstrate applicability of this understanding to an industrial process, fibres were spun from the dopes made by incorporating these additives and tracked for processability (by pressure tracking during spinning) and quality of fibres made.

This study can very well be extended to other functional product developments, where an understanding of interfacial interactions of specific additives and cellulose and their stabilisation using surfactants is critical.

Crystal Structure of 1-(2,4,6-Trichlorobenzoyloxy) Benzotriazole (TCB-OBt): Observation of Uncommon Intermolecular Oxygen-Oxygen Interaction and Synthetic Application in Amidation

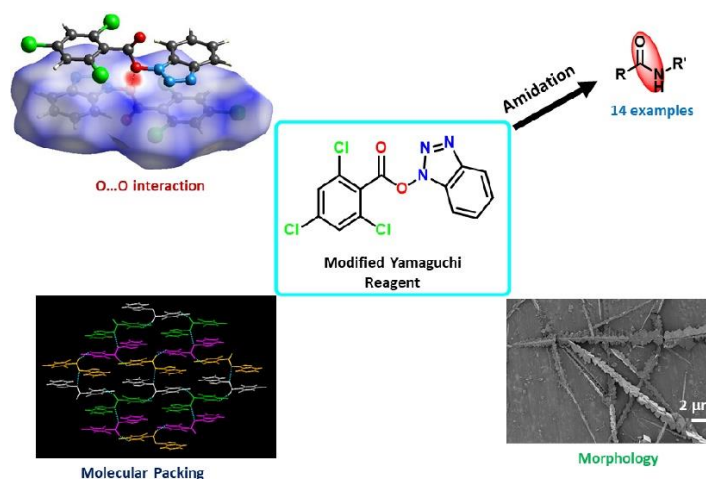
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The formation of supramolecular solid-state architectures of organic molecules has a remarkable impression on crystal engineering and supramolecular chemistry. Various non-covalent interactions such as hydrogen bonding, π - π stacking, C-H... π interaction, electrostatic interaction, and van der Waals interaction are main stabilizing forces for supramolecular structure formation.¹ Other Secondary bonding interactions (SBIs)² like chalcogen-chalcogen interaction, also play a considerable role in this process. Amide moiety is present on various natural products, active pharmaceutical components, polymers, and other biologically significant molecules. Yamaguchi *et al.* first developed Yamaguchi reagent TCB-Cl, useful for the effective formation of esters and lactones.³ Herein, we investigated the supramolecular assembly of a Modified Yamaguchi Reagent TCB-OBt. Each molecule is interconnected through novel O...O interaction, π - π stacking, and aromatic C-H...O interaction. Hirshfeld surface analysis confirmed the existence of uncommon O...O interaction. TCB-OBt crystallized in the O-substituted desmotropic form. DFT calculation suggested the O-substituted form is more stable than the N-substituted. Morphology analysis indicated the formation of a fantastic well organized, continuous block-shaped system. Furthermore, the designed reagent works as an efficient activating reagent for amide bond formation with good yield in mild reaction conditions. This reagent may further be applicable for many other organic transformations and material science.

Keywords: Supramolecular structure, Modified Yamaguchi Reagent, O...O interaction, amidation



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Unfolding of Tryptophanoctyl Ester and Elastic Deformation of Host Micelles via $RR'3N+\dots\pi$ Interaction: Conceivable Relevance to Wrapping Process of Receptor Mediated Endocytosis

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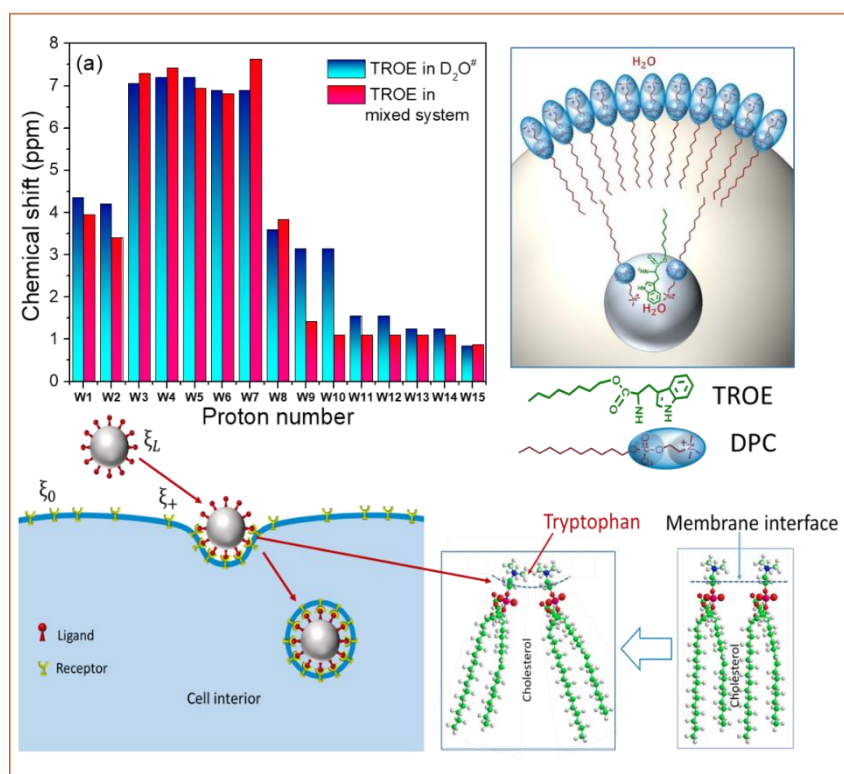
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The interfacial properties of the mixed amphiphiles are modified by a stronger cation- π interaction between the quaternary ammonium head group of cetyltrimethylammonium bromide (CTAB) and the π -face of tryptophanoctyl ester (TROE), compared to the tyrosine analogue (TYOE). This eventually triggers a morphology transition through elastic deformation of the spherical micelles of CTAB to cylindrical/wormlike micelles. The unfolding of TROE and the molecular interactions in the nanoenvironment is recognized by NMR spectroscopy and the physical characteristics of the entangled wormlike micelles are investigated by high resolution transmission electron microscopy (HRTEM), whereas the complex fluidic feature is examined by dynamic rheological measurements. Morphology tuning of the soft nanoaggregates of zwitterionic dodecylphosphocholine by the tryptophan analogue via choline- π interaction has unique biological consequences significant in facilitating endocytosis of a virion/nano particle (NP) in terms of a quantitative model.



Dispersion of Essential Oil Extracted from Peels of Mandarin Orange in Aqueous Isopropanol/ Isopropanol-TritonX-100 Mix Media

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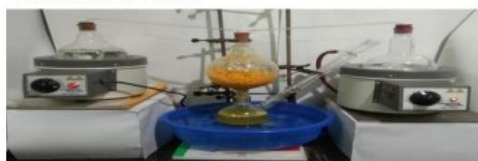
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The essential oil present in the peels of *Citrus reticulata* (common name - mandarin orange) harvested from the Tamenglong District of Manipur has been extracted using semi-mechanical method as well as modified hydro-distillation unit designed and assembled in the Laboratory. The standard hydro-distillation method gave colorless essential oil but our modified method gives essential with the orange color and aroma. However, the essential oil obtained using the semi-mechanical method gave pure oil with intense color and aroma. The average yield of the essential oil extracted was found to be as high as 4% depending on the quality of the peel and the method of extraction. The major chemical components of the essential oil have been identified based on GC/MS and spectroscopic data. The density, viscosity, saponification value, acid value, etc. of the oil have been determined. The dispersibility of the essential oil in water in presence of isopropanol, TritonX-100 or isopropanol-TritonX-100 mix media has been analyzed from the ternary phase diagrams of the components. Formation of gel in aqueous TritonX-100 media was observed with clear separation of crystal-like phase with intense orange color. The microemulsion of the essential oil in aqueous isopropanol with or without the surfactant and the gel showed good stability.

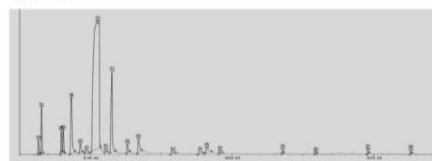
Keywords: Essential oil; Hydro-distillation; GCMS; Microemulsion.

Graphical schematic representation of the work in brief:

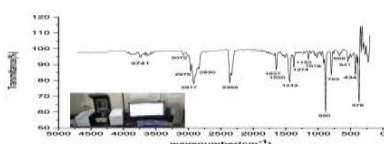
1) Distillation unit



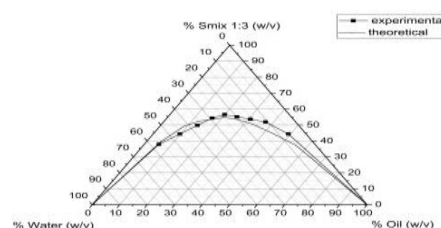
3) GCMS



2) FTIR:



4) Microemulsion



Detailed report and information will be present in the poster presentation

References:

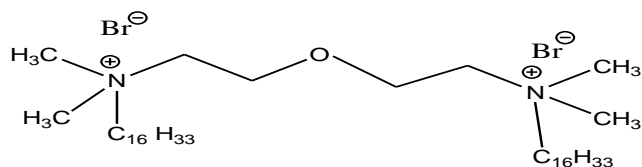
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Mixed Surfactant System as Additive for the Stabilization of Coal-Water Slurry

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The present work reported the interaction between cetyl trimethyl ammonium bromide (CTAB) and a cationic Gemini surfactant with dimethylammonium head groups and an ethoxyethyl spacer (Molecular structure-1) for the stabilization of concentrated coal-water slurry (CWS). The mixed system of the Gemini surfactant (C16-s-C16) and cationic surfactant (CTAB) was selected to disperse the concentrated CWS formed from Talcher coal containing 39.02 ash. The gemini-CTAB surfactant mixture showed synergistic activity in comparison to the single system of CTAB as indicated by decrease in the experimental CMC in comparison to ideal CMC predicted theoretically from the Clint equation. At 1:4 ratio the gemini-CTAB surfactant mixture showed maximum synergism, and hence the dispersant with this ratio was used for the stabilization of the slurry. On analyses of the adsorbent dose, coal load, variation of pH, temperature, static stability test of the CWS formed in presence of the mixed surfactant was found to have good slurriability and better stability. The CWS shows shear-thinning characteristics, following the Bingham plastic rheological model. In summary, the prepared mixed surfactant system can perform as an additive for stabilizing the CWS formed from low rank coal.



Molecular structure of Gemini surfactant

Key words: Coal-water slurry, synergism, slurriability.

Synthesis, Characterization and In-Vitro Antiproliferative Assays of Dithiocarbazate Based Compounds

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A series of heterocyclic based dithiocarbazates compounds L1-L4 *N'*-(1-methyl-1*H*-imidazol-2-ylmethylene)-hydrazinecarbodithioic acid methyl ester (**L1**), *N'*-(1-methyl-1*H*-imidazol-2-ylmethylene)-hydrazinecarbodithioic acid benzyl ester (**L2**), *N'*-[1-(1*H*-benzimidazol-2-yl)-ethylidene]-hydrazinecarbodithioic acid methyl ester (**L3**) and *N'*-[1-(1*H*-benzimidazol-2-yl)-ethylidene]-hydrazinecarbodithioic acid benzyl ester (**L4**) has been prepared and characterized by various spectroscopic techniques using SXRD, NMR, UV-Vis, mass spectrometry, IR and thermal analysis aiming to evaluate its cytotoxic activity to face the challenge of multi drug resistance in treatment of cancer. Compound **L1** and **L3** adopt a planar conformation and crystallizes as orthorhombic crystal system in P 21 21 21 space group and as monoclinic in P 21/c. MTT assay against H520 (Squamous cell lung carcinoma) cell reveals that N-Methyl imidazole based dithiocarbazates shows lower cytotoxic value (IC₅₀ value=15 and 17) than benzimidazole (IC₅₀ value= 33 and 40) containing moieties and could be a better choice for chemotherapeutic agent. The HOMO-LUMO energy gap of the four compounds **L1-L4** is 4.2, 3.94, 3.95 and 3.87 eV respectively.

Keywords: Dithiocarbazates; XRD; MTT Assay;

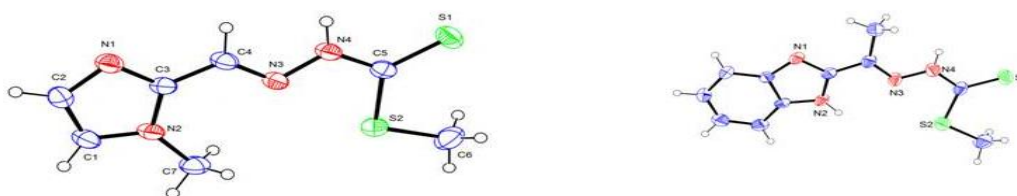


Figure 1. ORTEP diagram of L6 and L8 with ellipsoids at the 30% probability level.

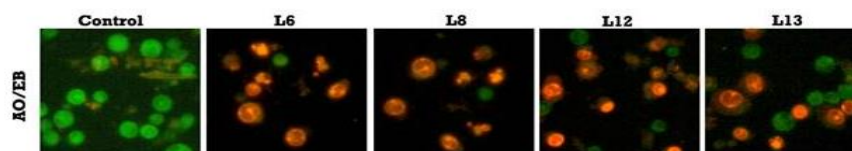


Figure: 2. Ao/Eb: Control, L6, L8, L12, and L13, treated cells. Green colour cells are live cells and Red colour cells showing apoptotic morphology

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Chaotropic Effect of Ions on the Aggregating Propensity of Whitlock's Caffeine Molecular Tweezer

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Molecular Tweezers feature the first class of supramolecular receptors to emerge as an effective therapeutic candidate with exquisite binding specificity. Its inclination however, to self-aggregate by mutual π - π stacking of their aromatic arms, diminishes their efficacy. Therefore, following up on studies since the discovery of the Hofmeister series, the notions of ion-specificity effects are utilized on the tweezer moieties. The impact of three aluminium salts bearing the anions, Cl^- , ClO_4^- and SCN^- are investigated on the association propensity of Whitlock's molecular tweezers. The comparative investigation is conducted employing a series of molecular dynamics simulations of five tweezer molecules in pure water and the three salt solutions, at two concentrations each. RDF plots, SASA and cluster analyses display a reduction in the aggregation proclivity of the receptors and increase in salting-in ability from Cl^- , ClO_4^- to SCN^- . Preferential interactions and tetrahedral order parameters unveil the underlying mechanism, by which the anions alter the solubility of hydrophobic molecules. Overall, we observe that anions inhibit aggregation of the tweezers through different mechanisms, ClO_4^- ion impart an effect by modifying the water structure, while, SCN^- engage in direct interaction with specific tweezer sites. Cl^- being the most charge-dense, experience stronger hydration and thereby, impart negligible salting-in effect.

Keywords : Hofmeister effect; molecular tweezer; salting-in

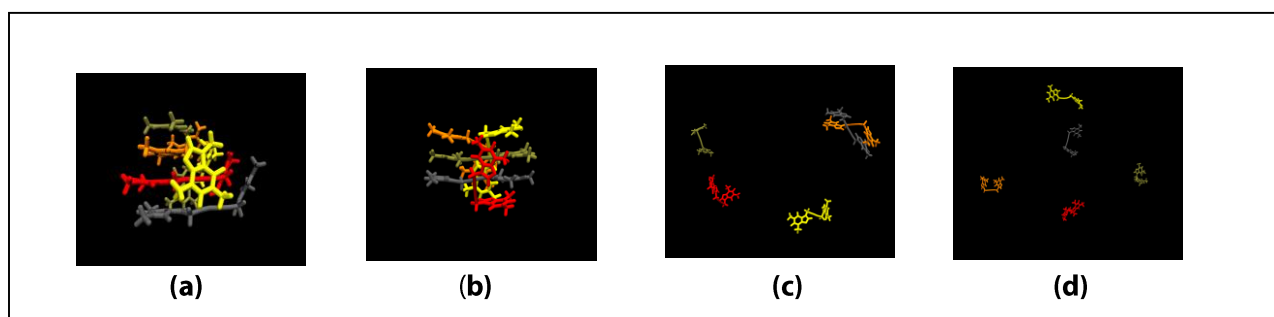


Figure 1: Snapshots captured after 300 ns simulation (a) pure water system, (b) 2 M AlCl_3 system, (c) 2 M $\text{Al}(\text{ClO}_4)_3$ system, (d) 2 M $\text{Al}(\text{SCN})_3$ system.

Tolerant and Hard Superhydrophobicity: Restricting Physical Deformation

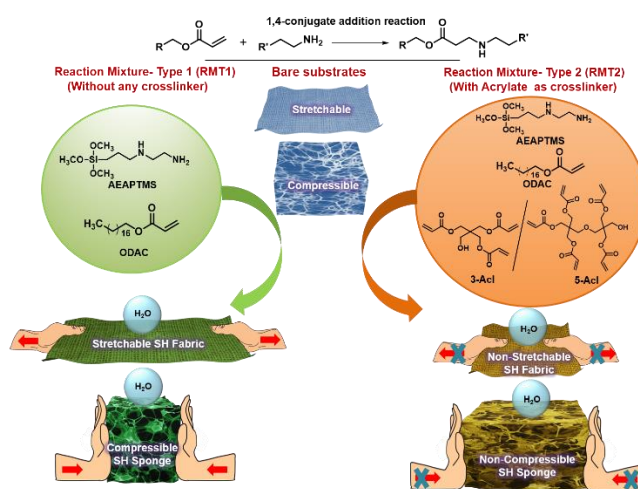
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Lotus leaf-inspired superhydrophobicity emerged as a prospective avenue for developing various functional materials¹. But the durability of such nature-inspired artificial materials remains a significant concern and thus restricts its future applications in outdoor settings. Multiple strategies have been introduced in the last few years to develop abrasion tolerant and mechanically durable superhydrophobic coatings.² Although some of these seminal reports achieved durable superhydrophobic coatings on rigid substrates, most reported approaches followed complex fabrication processes or required sophisticated setups.³ Moreover, the previously reported strategies could not tailor the mechanical properties of the soft and geometrically complex (fibrous and porous) substrates. In this work, we have reported facile 1,4-conjugate addition reaction under ambient conditions between selected reactants, i.e. [3-(2-aminoethylamino)propyl]trimethoxysilane (AEAPTMS) and octadecyl acrylate (ODAc), in the presence and absence of crosslinker molecules [pentaerythritol triacrylate (3-AcI) or dipentaerythritol penta-acrylate (5-AcI)] to develop either non-deformable or deformable (compressible/stretchable) superhydrophobic coatings on selected soft and deformable respectively, as shown in Schematic. The compressive and tensile moduli of the selected soft substrates increased by $2.2 \times 10^4\%$ and $1.8 \times 10^4\%$, respectively, after the deposition of the appropriate reaction mixtures. Moreover, the integration of the crosslinkers in the reaction mixture provided a facile basis to resist the physical erosion/rupture of the selected soft substrates under severe abrasive conditions. Hence this current approach is likely to open up the possibilities for using prospective bio-inspired wettability in different and relevant outdoor applications in the future.

Keywords: Superhydrophobicity, Cross-linker, non-deformable, tolerant.



Scheme: Schematic illustration for the preparation of deformable and non-deformable superhydrophobic materials.

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Peptide Functionalized Carbon Dots based Fluorescent Sensor for Detection of Lipopolysaccharide

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Bacterial Lipopolysaccharides are known to be frequent contaminants derived from biological preparations and their removal from such solutions remains a very challenging task for bioprocess engineers. Carbon nanodots (C-dots) have been found to generate enormous excitement for the detection of such biological toxic molecules because of their superiority in water solubility, chemical inertness, low toxicity, ease of functionalization and resistance to photobleaching. Here, we synthesize carbon nanodots (C-dots) using a single-step procedure based on microwave heating of aqueous solution of citric acid and urea, which is further functionalized with a specific peptide. The structure and properties of the resulting materials are studied using a series of spectroscopic techniques viz., UV, FTIR, and Fluorescence. The small size of the isolated carbon dots along with their strong absorption in the UV and their excitation wavelength-dependent fluorescence render them ideal candidates for biomedical sensing of endotoxin (lipopolysaccharide). The fluorescence of the functionalized carbon dots is quenched upon specific interaction of peptide with lipopolysaccharide. Thus, this approach offers a complete and versatile toolbox for rapid detection of biological toxic molecule in clinically relevant matrices.

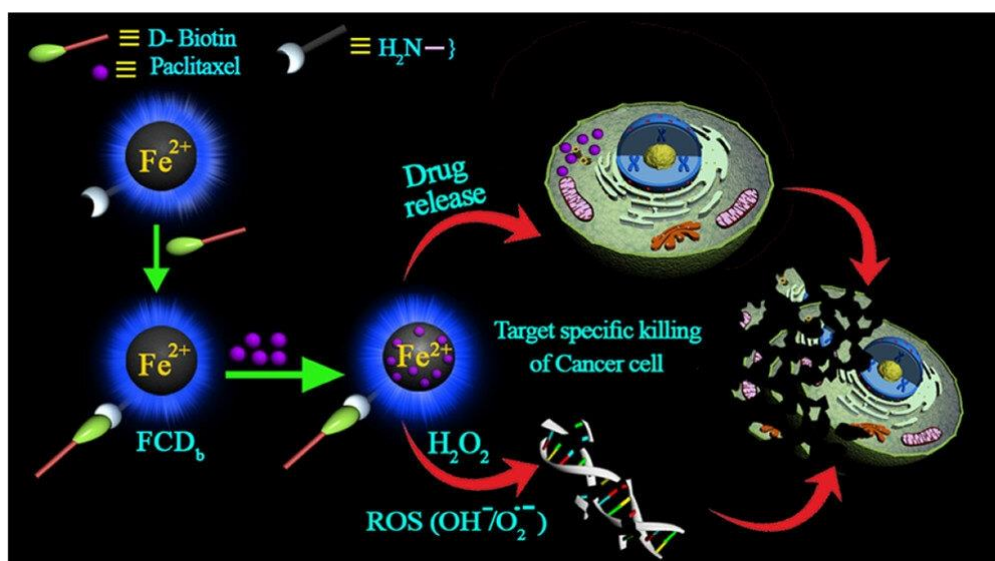
Paclitaxel-Loaded Biotinylated Fe²⁺-Doped Carbon Dot: Combination Therapy in Cancer Treatment

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The present research work delineates the design and preparation of covalently tailored biotinylated Fe²⁺-doped carbon dots¹ (FCD_b). The FCD_b was successfully used as a pro-drug activator², diagnostic probe, and target-specific delivery vehicle for anticancer drug paclitaxel³ in pro-drug-free drug combination therapy⁴ of cancer treatment. Fe²⁺-doped carbon dot was synthesized via the hydrothermal method (FCD). The surface of FCD was covalently modified with cancer cell targeting ligand biotin (FCD_b). Microscopic and spectroscopic methods were used to characterize aqueous soluble FCD and FCD_b. Both FCD and FCD_b emit blue fluorescence under UV light irradiation. FCD and FCD_b can effectively sense H₂O₂ by fluorescence quenching as well as activate H₂O₂ (pro-drug), which oxidatively damage the DNA through the generation of reactive oxygen species (ROS: superoxide (O₂^{•-}), hydroxyl radical (•OH), etc). Both FCD and FCD_b were utilized as selective cellular markers for cancer cell B16F10 owing to their high H₂O₂ content, which was more distinct in the case of FCD_b due to the overexpression of biotin receptor in cancer cell. Anticancer drug paclitaxel (PTX)-loaded FCD_b (FCD_b - PTX) was employed for the selective killing of B16F10 cancer cells. This pro-drug-free drug formulation (FCD_b -PTX) exhibited ~2.7- to 3.5-fold higher killing of B16F10 cells mostly via early as well as late apoptotic path in comparison to noncancer NIH3T3 cells through the synergistic action of ROS (generated from H₂O₂ in the presence of FCD_b) and anticancer effect of PTX. Hence, this newly developed FCD_b -PTX can act as a potential theranostic agent in the domain of combination therapy of cancer treatment.

Keywords: Fe²⁺-doped carbon dots, pro-drug-free drug, combination therapy, paclitaxel.



Pictorial presentation of paclitaxel loaded biotinylated Fe²⁺ doped carbon dot (FCD_b) as a theranostic agent in pro-drug-free drug combination therapy.

References:

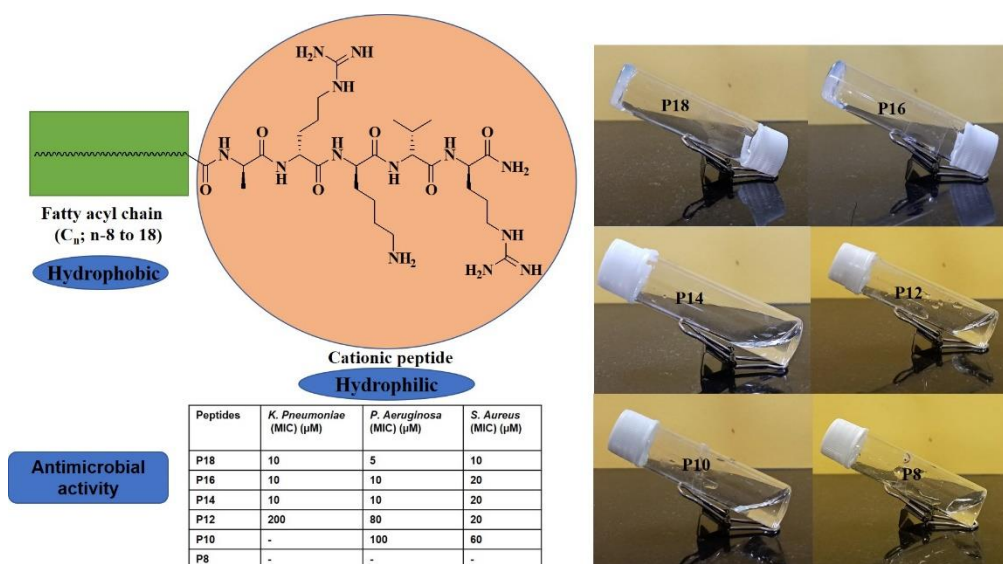
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Effect of the Fatty Acyl Chain Lengths in the Antimicrobial and Assembling Abilities of Lipopeptides

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Extensive use of antibiotics leading to antibiotic resistance and ever-growing threats from drug-resistant bacteria have demanded the development of alternate antimicrobial agents¹. Antimicrobial peptides (AMPs) are a class of molecules that have a wide spectrum of activity against bacteria, viruses, fungi etc.² Loss of activity under high salt concentrations short half-life and toxicity against mammalian tissues are some of the bottle necks that limit their application in the field of pharmaceuticals³. In the present study, we have designed lipopeptides with various lengths of fatty acyl chain, to study effect of the later on the antimicrobial and assembling properties of the former. Lipopeptides with longer chain length formed hydrogel in phosphate buffer at pH 7.4 with fibrillar network structure and exhibited antimicrobial potency against ESKAPE pathogens like *Pseudomonas Aeruginosa*, *Staphylococcus Aureus* and *Klebseilla Pneumoniae* with an MIC in the range 5-10 μM . The active lipopeptides were salt-tolerant, non-cytotoxic and protease resistant in nature. Upon assembling into gel the active lipopeptides lost their antimicrobial activity. This might be attributed to the unavailability of the peptide molecules to interact with the microbes due to strong intermolecular association among the peptide molecules themselves.



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Chitosan Hydrogels with Embedded Dually Thermo- and pH-responsive Microgels as a Potential Carrier for Controlled Release of Drugs

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Herein, we report a novel strategy based on chitosan (CS) hydrogels and dually temperature- and pH-responsive poly(N-isopropylacrylamide-co-methacrylic acid) (PNIPAM-co-MAA) microgels to facilitate long-term drug delivery of a model drug, moxifloxacin (MFX). In this protocol, first, the microgels were prepared by free radical precipitation copolymerization and subsequently, these carboxyl-group-rich soft particles were incorporated inside the hydrogel matrix using an EDC-NHS amidization method. Interestingly, the resulting microgel-embedded hydrogel composites (MG-HG) as a double barrier system largely reduced the drug release rate and prolonged the delivery time for up to 68 h, which was significantly longer than that obtained using microgels or hydrogels alone (20 h). In account of dual-responsive features of the embedded microgels and the variation of water-solubility of drug molecules as a function of pH, MFX could be controllably released by adjusting the temperature and pH of the delivery medium. The release kinetics followed a Korsmeyer-Peppas model and the drug delivery mechanism was described by Fickian diffusion. Both the gel precursors and hydrogel composites exhibited a low cytotoxicity toward mammalian (HeLa and HEK-293) cells and no undesirable hemolytic activity up to a certain higher concentration, indicating an excellent biocompatibility of the materials. Thus, the unprecedented combination of modularity of physical properties caused by soft particle entrapment, unique macromolecular architecture, biocompatibility and general utility of the stimuli-responsive polymers offers a great promise to use these composite materials in drug delivery applications.

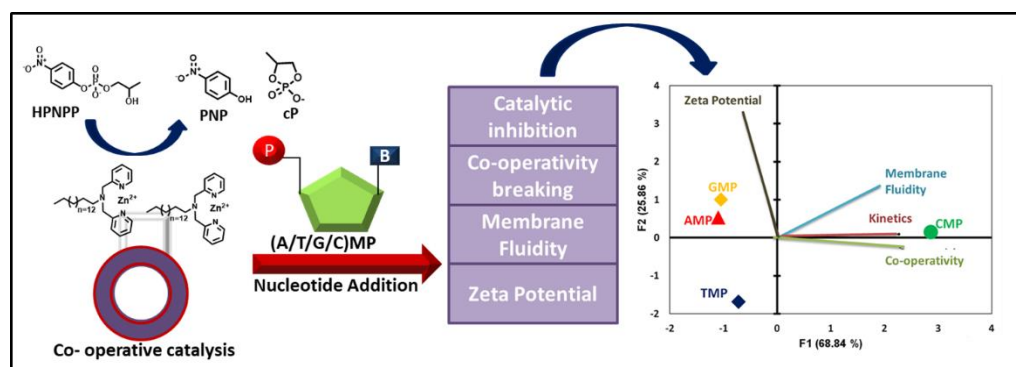
Patterning Nucleotide-Mediated Self-Assembly by Coalescing Catalytic Co-Operativity and Membrane Properties

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Each nucleotide play a specific role in biochemical pathways as - chemical messenger, coenzymes, energy storage molecule etc. apart from their eventual role in nucleic acid translation or transcription. Supramolecular chemists are interested in manufacturing unique nucleotide receptors by developing functional dynamic assemblies for biosensors, life-like complex systems, and other applications, utilising both nucleobase specific receptors and anionic phosphate moiety. In recent literature reports, nucleotides have been used as fuel to control the dynamic assembly process in a synthetic system, mimicking complex biochemical processes, like - actin or microtubule dynamics.¹ However, patterning of nucleotide-regulated synthetic self-assembled systems where catalytic ability of the system gets altered by the specific input of nucleotides correlated with other functional and structural parameters, remains unexplored.^{2,3} Herein, we explored nucleotide-mediated changes in catalytic properties of a substrate-driven cooperative self-assembly with the changes in membrane fluidity and charges. In this case, the micelle-like aggregate of a metallosurfactant converted to vesicle-like aggregate upon introduction of the RNA-model substrate, 2-hydropropyl-4- nitrophenyl phosphate (HPNPP) or/and the nucleotides.⁴ The native co-operative nature of the catalytic response was analysed in presence of nucleotides and correlated with changes in membrane polarity and charge. Finally, the discriminating pattern among all nucleotide monophosphates mediated changes in self-assembled structural assembly has been achieved using principal component analysis (PCA).

Keywords: Self-assembly, co-operative catalysis, Membrane Fluidity, Membrane Charge.



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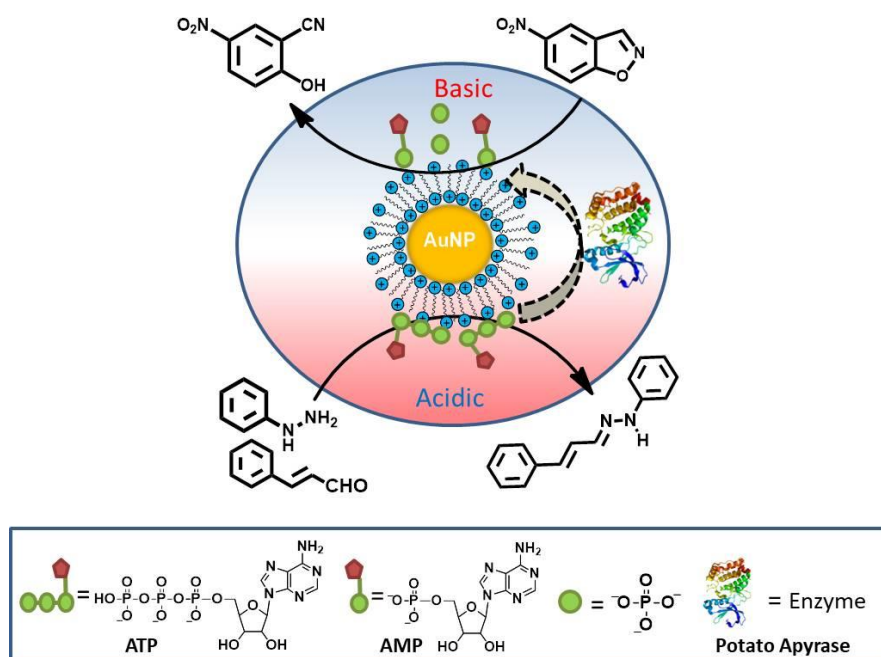
Catalytic Switch Mediated by a Bio-catalyst

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To build a novel sensing and catalytic system, monolayer protected gold nanoparticles are emerging as a class of molecular systems having potential applications in molecular recognition, catalysis, signaling, and adaptation as they are derived entirely from the organic monolayer rather than the inorganic support. It is foremost criterion to incorporate adaptive and dynamic behavior in a catalytic system to gain nature like functionality and generating physiologically relevant catalyst. Recently, we have developed a CTAB-capped cationic gold nanoparticle (GNP) based catalytic system which can be modulated for its performance by changing the number of phosphate groups (negatively charged group) in self-assembling units (AMP/ADP/ATP). As ATP having three phosphate groups can interact more strongly with the cationic surface as compared to AMP due to multivalent interaction. Due to stronger interactions of ATP with nanoparticles, the surface pH of the nanoparticles turns out to be acidic from basic while in the presence of AMP, the pH of the nanoparticles surface remain unchanged i.e. basic. Further, we have used these conditions to perform two different reactions, one which is favorable in acidic conditions (i.e., Hydrazone formation) and other one in basic conditions (i.e., Proton transfer, Kemp Elimination). Apart from this, we have also modulated the pH of the nanoparticles surface by using an enzyme named, Potato Apyrase in temporal manner and hence the selectivity of the nanoparticle catalytic system towards the two different reactions have been modulated.

Keywords: multivalent interaction; adaptive; dynamic; temporal manner.



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Aliphatic Diamine Fuelled Polarity-driven Transient Self-assembly and Disassembly-mediated Harvesting of Smart Materials with Versatile Applications

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A well-recognized chromophore such as pyrene offers ample opportunities to construct organic nanostructures *via* self-assembly which can remarkably tailor their optoelectronic properties.¹⁻³ Inspiringly, in this contribution, we have developed aliphatic diamine/ polyamine (AD/ AP) fuelled a reaction-based strategy to introduce self-assembly and disassembly properties of pyrene-AD/ AP conjugates. Upon reaction of pyrene dianhydride with AD/ AP, the system creates a highly polar transient excimer species *via* ground state dimer formation which further undergoes disassembly to generate discrete monomers in non-polar solvent. The alkyl chain length between two terminal amine groups in AD/ AP skeleton also plays a crucial role on tuning the rate of assembly and disassembly process. The open conformation of the conjugate is primarily responsible for demonstrating such phenomenon in solution. The phenomenon has been established by various spectroscopic and microscopic techniques. Finally, the blue-emissive monomeric conjugates have displayed its potentiality as solid-state emissive material as well as in live-cell imaging.

Keywords: Pyrene, Self-assembly and disassembly, Solid-state emission, Bioimaging

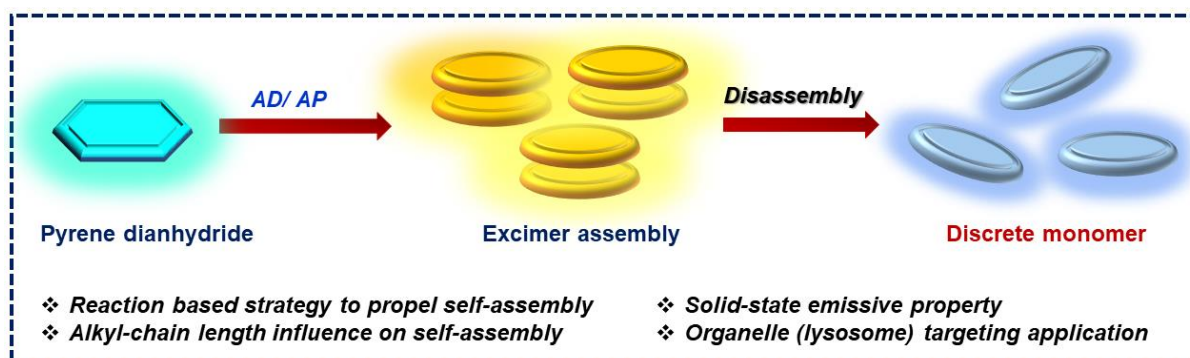


Figure 1. Schematic representation of pyrene-based self-assembly and disassembly

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Hydrolysis of N- [2-hydroxynaphthylidene]-(6)-Substituted-2-aminobenzothiazoles in Aqua-Organic Systems**Sagarika Panigrahi^{a*} and Pramila.K.Misra^{b*}**^a Lokadrusti College of Advanced Technology, Khariar, Nuapada-766107, Odisha, India^bCentre of Studies in Surface Science and Technology, School of Chemistry, Sambalpur University, Jyoti Vihar-768019, Odisha, India

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The hydrolysis of some biologically active Schiff bases N-[2-hydroxy-1-naphthylidene]-2-amino-X-substituted-benzothiazoles (X= H, Me, NO₂) has been done in presence of cationic surfactant CTAB, anionic surfactant SDS and nonionic surfactant TX-100. The rate of hydrolysis was measured spectrophotometrically with variation pH in presence of the aqua-organic systems (60:40v/v) 1,4-dioxan-water system. Addition of organic solvents break down the spherical structure of micelle, it has not been possible to say as to the nature of the surfactants systems in a solvent containing such a high percentage of 1,4-dioxane. Therefore, an attempt has been made to study the kinetics in this solvent system with a view, to examine, if the surfactant behaves as a strong electrolyte or behave as strong aggregates. The pH rate curve is found to have 4 distinct regions having different mechanistic path influencing by the attacking species H₂O or OH⁻ and the environment of the medium, pH etc. The kinetic and thermodynamic pK values of the corresponding conjugate acid and the anion form of the Schiff bases were calculated both in absence and presence of surfactant. The shift in pK was analogous to the shift of pK values of the dissociating groups in the enzymatic systems due to the different environment, available to it.

Self-Assembly and Desulfurization of Amphiphilic Chemosensors in Turn-ON Mercury Sensing in Aqueous Media

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A water-soluble substituted thiourea amphiphile detects mercury with a Turn-On emission signal. Desulfurization-directed mercury detection in water has been resolved with spectral studies. Noteworthy, water-insoluble substituted thiourea collectively with hydrophobic chain renders sensing in aqueous media. The amphiphilic thiourea shows appreciable selectivity and sensitivity among other cations and heavy metals, contrary to its control compound. The asymmetric tripod is capable of self-assembling into ribbon-like morphology in aqueous media. Both assembly and disassembly process has been outlined by microscopic analysis. The analytical utility of the tripod has been probed through real water samples and soil testing. Moreover, the Hg-ensemble selectively recognizes H₂S viz; sulphide ion in water and rendering a substantially low detection limit of 0.5ppm. Realistically, paper strips are set for the fluorimetric visualization of both the toxins.

Keywords: Self-assembly; Amphiphilic chemosensors; Turn-On Mercury sensing.



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Bi-Directional Feedback Controlled Transience in Cucurbituril Based Tandem Nanozyme

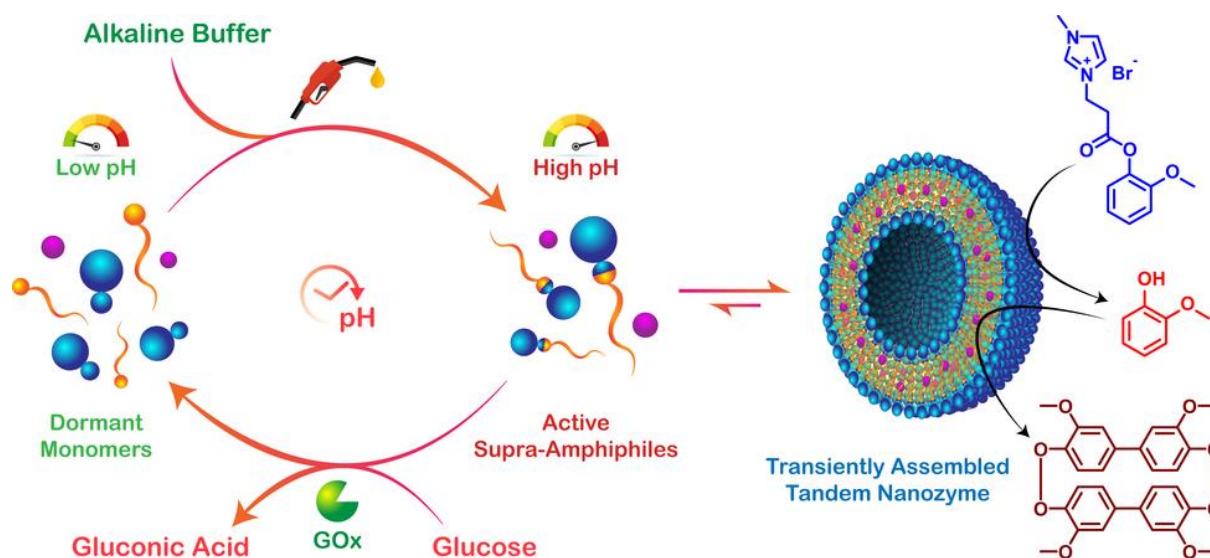
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Life is fuelled by multi-enzymatic tandem processes that display unmatched catalytic efficiencies owing to certain features of the biological reactors such as compartmentalization, nano-confinement, and out-of-equilibrium dynamics. With an attempt to match such natural catalytic systems, herein, we present a chemoenzymatic pH clock¹ mediated transient assembly of a vesicular nanozyme. Distinct confinement of two catalytically discrete units, Histidine groups on the periphery and hemin in the lipid bilayer, results in an efficient hydrolase-peroxidase tandem catalysis in a temporally controlled fashion. The pH clock, constituted by alkaline TRIS buffer (promoter) and glucose oxidase (GOx) catalysed oxidation of glucose, steers the transience in an asymmetric fashion. Alkaline TRIS buffer enhances the pH of the system and triggers the formation of imine linked Supramolecular Peptide Amphiphiles (SPAs) that further assemble into vesicles. On the other hand, oxidation of glucose produces gluconic acid, which dissipates the nanozyme, and H₂O₂ which feeds the peroxidase catalysis. The transiently assembled nanozyme protected the activity of the catalytic units, displayed substrate specificity and catalytic reproducibility over multiple fuelling cycles.

Keywords: transient self-assembly, nanozyme, tandem catalysis, peroxidase



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Supramolecular Assemblies of Boc-Protected Dipeptides and its Structural Features in Crystalline State

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Molecular self-assembly of small di- or tri-peptides to form various micro- or nano-scale structures has gained important applications in Bioorganic chemistry, material sciences, and medicinal chemistry.¹ Supramolecular non-covalent interactions stabilize the secondary structure of peptide or protein. Herein, we designed an alternating L/L and L/D amino acid-containing dipeptides Boc-L-Ile-L-Phe-OMe (1), Boc-L-Ile-D-Phe-OMe (2), Boc-L-Ile-L-Phg-OMe (3), and Boc-L-Ile-D-Phg-OMe (4), and investigated their supramolecular self-assemblies. The presence of extra methylene (-CH₂-) group on the side-chain of C-terminal Phe of 1 causes a significant deviation of molecular arrangements from that of 3. While the molecules in 1 self-assemble to form a single helix-like architecture, the molecules in 3 self-associate around a water molecule to form a cylinder-like structure in the crystalline state. On the other hand, the observed supramolecular arrangements of 2 and 4 are similar, but deviate from that of 1 and 3, due to the chirality difference. Peptides 2 and 4 exhibit a discontinued double helix-like structure in the crystalline state. While 1 and 3 self-associate to form helical ribbon-like and nano tube-like structures, respectively, both 2 and 4 form nanorod like structures in solution.²

Keywords: Dipeptide; Crystal structure; Self-assembly.

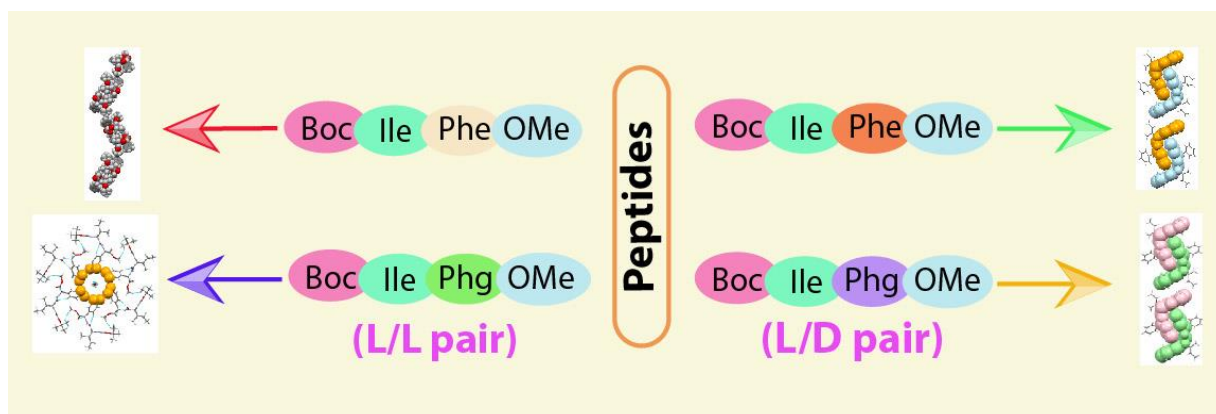


Figure. Molecular self-assembly in crystalline state.

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Designing Cellulose Based Functional Materials for Green Energy Related Technology and Biotechnological Application**Sourav Sen**, Kamalakannan Kailasam* and Sangita Roy*Institute of Nano Science and Technology, Sector-81, Manauli,
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In recent years, due to high energy consumption in the building sector and subsequent environmental issue, environment-friendly and cost-effective thermally insulating materials are on high demand to improve the energy efficiency of the buildings. Current commercially available thermal insulating material (polystyrene) always put a challenge due to their fragile nature, non-biodegradability and poor insulating performance. To this end, biomass derived aerogels are receiving more interest as renewable and sustainable insulating materials. In this work, we have developed a facile strategy of synthesizing nano-fiber cellulose from biomass derived wood pulp as a cost-effective starting material by TEMPO-oxidation and incorporated iron oxide nanoparticles to synthesize nanohybrid. Interestingly, in these nanohybrids, the functional attributes like mechanical strength and flammability were improved to a greater extent, which overcomes the limitations of the commercially available thermal insulating materials in terms of their stability and durability. Most importantly, the nanohybrid demonstrated very low thermal conductivity as low as 0.024 W/mK, indicating better insulating potential of these nanohybrids as compared to other conventional insulating materials. Furthermore, the in-situ fabrication potential of these natural polymer will be highlighted towards synthesizing cellulose metal nanoparticles hybrids, which can be further explored for photocatalysis, water purification as well as photodynamic therapy for cancer treatment.

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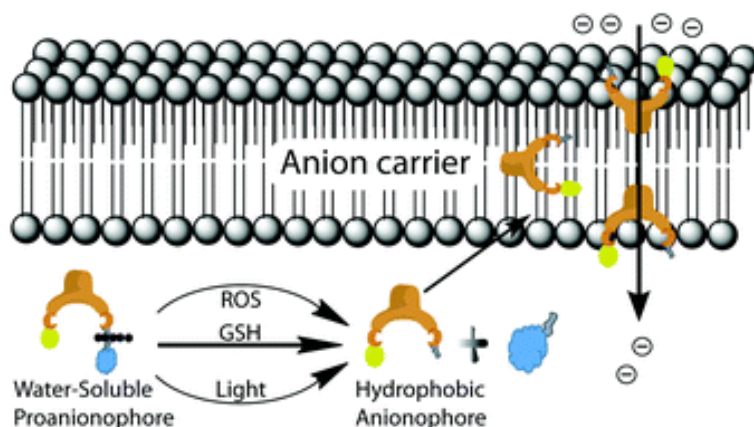
Multi-stimuli Controlled Release of a Transmembrane Chloride Ion Carrier from a Sulfonium-Linked Procarrier

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In recent times, anion transporters have received substantial consideration due to their ability to disrupt the ionic equilibrium across membrane bilayers. While numerous Cl^- ion transporters were developed for channelopathies, unfortunately, poor aqueous solubility precluded their bioapplicability. Herein, we demonstrate the development of a multi-stimuli activatable anion transport approach to induce regulated transport of Cl^- ions across membranes under specific conditions. The sulfonium-based procarrier was initially inactive, but the transmembrane transport of Cl^- ions was activated in the presence of stimuli such as glutathione (GSH), reactive oxygen species (ROS) and light. The release of the hydrophobic anionophore from the aqueous-soluble procarrier under specific conditions leads to the successful transport of Cl^- ions. Under physiological conditions, these anion carriers follow an antiport exchange mechanism to transport Cl^- ions across lipid bilayers. Such multi-stimuli activatable procarriers have great potential to combat various types of channelopathies, including cancer, cystic fibrosis, kidney stones, myotonia, and others.

Keywords: Procarrier; Multi-stimuli; Channelopathies.

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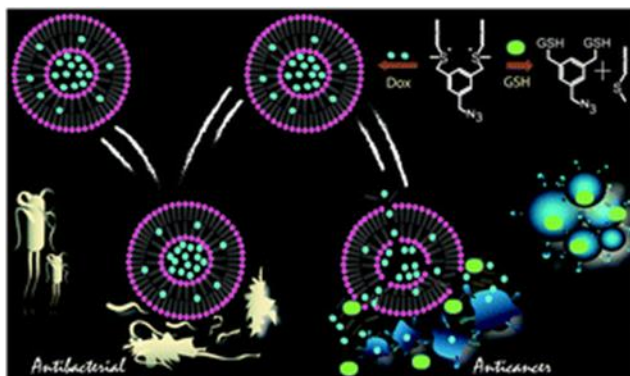
A stimuli-responsive anticancer drug delivery system with inherent antibacterial activities

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The delivery of drug molecules to specific cells through blood circulation system is one of the major impediments in pharmaceutical research. Advanced drug delivery systems including lipid-based nanoparticles are considered as promising tools to effectively transport a wide range of therapeutic agents to targeted cells with apposite therapeutic doses. Biodegradability, non-immunogenicity and others are the unique felicitous properties of lipid-based drug delivery systems. Recently, the stimuli-responsive drug delivery strategy has been considered as one of the practical approaches for cancer treatment. Significant changes in internal physiological conditions of the tumour microenvironment, have been used as stimuli for chemotherapeutic drug delivery applications. These stimuli cause a significant change in the chemical structure of the drug carriers due to the cleavage of their specific functional groups or the changes in their physicochemical properties, which instigate the release of encapsulated drug molecules in-or-around diseased cells. We describe a novel class of stimuli-sensitive sulfonium-based synthetic lipids, which exhibit several favourable biophysical properties of phospholipids. The potent sulfonium-based lipid was successfully disassembled by glutathione to release the encapsulated drug molecules in a controlled manner. The cationic lipid also showed lower cytotoxicity against mammalian cells and displayed moderate antibacterial activities.

Keywords: antibacterial activities; drug delivery; Lipid; stimuli-responsive.



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Dey, S.; Patel, A.; Raina, K.; Pradhan, N.; Biswas, O.; Thummer, R. P.; Manna, D. Stimuli-Responsive Anticancer Drug Delivery System with Inherent Antibacterial Activities. *ChemComm* **2020**, *56*, 1661-1664.

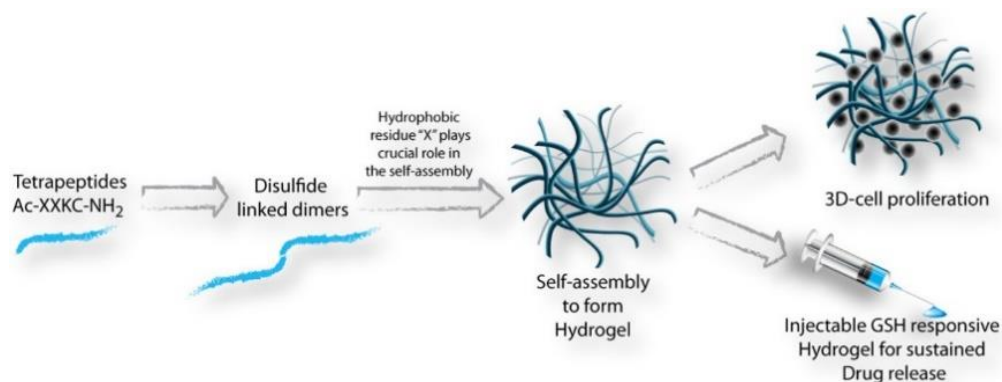
Smart Thixotropic Hydrogels by Disulfide-Linked Short Peptides for Effective Three-Dimensional Cell Proliferation

Sumit Chowdhuri, Amrita Saha, Bapan Pramanik, Saurav Das, Payel Dowari, Anindita Ukil, and Debapratim Das*

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There is significant interest in utilizing self-assembly in biomedicine to construct mimics of the extracellular matrix (ECM) for cell-culture applications. For this purpose, inspired from the previous work¹, we have prepared a series of short peptides having the basic unit 'Lys-Cys' ('KC') and a varying hydrophobic unit in N- terminal position. Cysteine acts as a redox unit for dimerization of the peptides by establishing a disulphide bond. However, these dipeptides are ineffectual in forming the hydrogel but depend on the acetyl unit's availability in the N-terminal positions in the peptides, AcFFKC and AcVVKC, to form independent self-supported hydrogels. The presence of H₂O₂ in the pre-gel solution accelerates the hydrogelation rate and enhances the stiffness of the hydrogel. The detailed rheological study revealed that both hydrogels are thixotropic. However, the hydrogel of Ac-FFKC-NH₂ is found to be more robust and more effective for biological applications. In addition, they are responsive to glutathione (GSH) due to the presence of disulfide linkages. A model drug release study in response to varying GSH concentrations indicates the hydrogel's possible use as an injectable local drug delivery vehicle. Three-dimensional cell proliferation is more effective than 2D, as it mimics the in vivo situation more closely, if not precisely. In the present study, we have shown that both differentiated RAW macrophages and undifferentiated THP-1 monocytes could increase significantly within the 3D matrix of the hydrogel. Thus, the hydrogel of Ac-FFKC-NH₂ has potential for application in localized drug administration and as a supporting biomaterial to study fundamental phenomena involving cell behaviour.²

Keywords: Peptide; Hydrogel; Cell proliferation; Extracellular Matrix.



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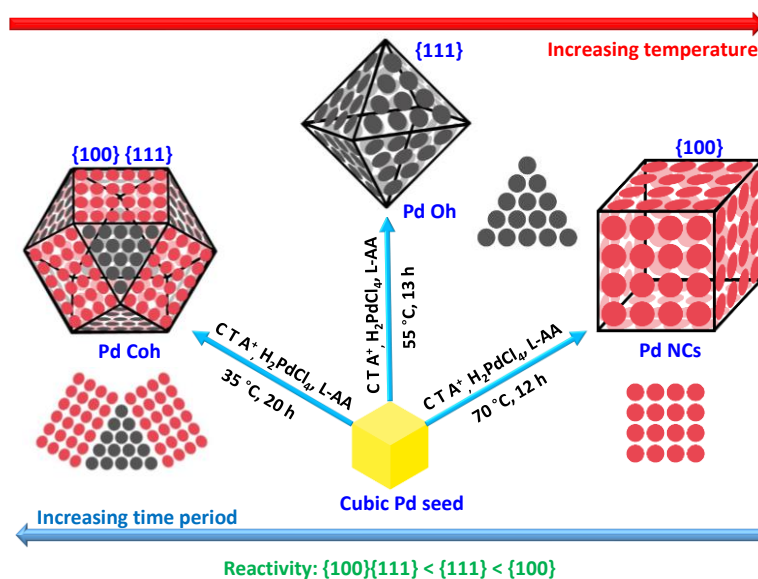
Facets Dependent Catalytic Activity of Pd Nanocrystals for the Remedy of Organic Pollutant: A Mechanistic Study

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Facet dependent catalytic activities of Palladium (Pd) nanocrystals have great significance in the field of catalysis. In this report, the robust seed-mediated synthesis method by taking Cetyl trimethyl ammonium bromide has been used to synthesize cuboctahedral (Coh), octahedral (Oh), and cubic Pd nanostructures. Optimizing the reaction time and temperature, the growth of nanocrystals directed along different low index planes such as {100} for Pd NCs, {111} for Oh and mixed planes of {100} and {111} assigned for Coh structure. To understand the role of different facets, nanocrystals were employed for the reduction of organic pollutant 4-Nitroaniline (4-NA) to 4-Phenylenediamine (4-PDA), and substituent effect of nitro ($-\text{NO}_2$) group such as 3-NA and 2-NA were studied. By keeping the total surface area of particles, the same, different volumes of nanocrystals were taken into account to carry out an accurate facet-dependent analysis. To extend the catalytic activity, degradation of cationic dye, Rhodamine B (Rh B), and anionic dye, Methyl Orange (MO) were studied. The reduction and degradation process were monitored through UV-Visible absorption spectroscopy. It was confirmed from the absorption spectra that the efficiency of Pd NCs was higher than Oh and Coh nanocrystals, which established the depiction of the best role of {100} planes out of the other two planes exposed on the surface. The catalytic trends of low index planes follow the order NCs {100} > Oh {111} > Coh {100} {111} for Pd nanocrystals was confirmed from the analytical model.



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Biodegradation of Waste Cooking Oil and Simultaneous Production of Rhamnolipid Biosurfactant by *Pseudomonas aeruginosa* P7815 in Batch and Fed-Batch Bioreactor Studies

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Biosurfactants are non-toxic, surface-active biomolecules capable of reducing surface tension (ST) and emulsifying interface at a comparably lower concentration than commercial surfactants. Yet, poor yield, costlier substrates, and complex cultivation processes limit their commercial applications. This study focuses on producing biosurfactants by *Pseudomonas aeruginosa* P7815 in batch and fed-batch bioreactor systems using waste cooking oil (WCO) as the sole carbon source. The batch study showed a 92 % of WCO biodegradation ability of *P. aeruginosa* producing 11 g L⁻¹ biosurfactant. To enhance this biosurfactant concentration, a fed-batch oil feeding strategy was opted to extend the stationary phase of the bacterium and minimize the effects of substrate deprivation. An enhanced biosurfactant concentration of 16 g L⁻¹ (i.e., 1.5 times of batch study) was achieved at a feed rate of 5.7 g L⁻¹d⁻¹ with almost 94 % of WCO biodegradation activity. The biosurfactant was characterized as rhamnolipid using Fourier transform spectroscopy (FTIR), and its interfacial characterization showed ST reduction to 29 ± 1 mN m⁻¹ and effective emulsification stability at pH value of 4, temperature up to 40 °C and salinity up to 40 g L⁻¹. The biosurfactant exhibited antibacterial activity with minimum inhibitory concentration (MIC) values of 100 µg mL⁻¹ and 150 µg mL⁻¹ for pathogenic *E. hirae* and *E. coli*, respectively. These findings suggest that biodegradation of WCO by *P. aeruginosa* in a fed-batch cultivation strategy is a potential alternative for the economical production of biosurfactants, which can be further explored for biomedical, cosmetics, and oil washing/recovery applications.

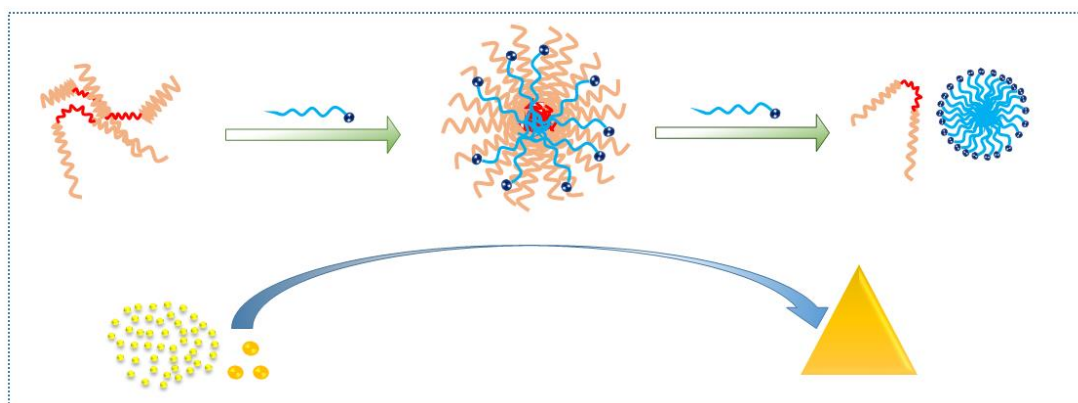
Keywords: Biosurfactants; Fed-batch bioreactor; Waste cooking oil; Antibacterial; Surface Tension

Photophysical Investigation of a Sub-Micellar Triblock Copolymer-Cationic Surfactant Aggregate for Gold Nanoplate Synthesis

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Surfactant assemblies are efficient medium for the synthesis of a variety of shape-controlled nanostructures. However, the requirement of large amounts of surfactants is detrimental to biological and medical applications. Herein, we optimized the size and interfacial packing of a sub-micellar aggregate of a triblock copolymer F127 (poly-(ethylene oxide)₁₀₁ (EO₁₀₁)–poly(propylene oxide)₅₆ (PPO₅₆)–PEO₁₀₁), and several cationic alkyl trimethylammonium surfactants at minute concentrations and demonstrated its feasibility in synthesizing gold nano-triangles.¹ We tracked various stages of the sub-micellar aggregate using an ultrasensitive photoacid 8-hydroxypyrene-1,3,6-trisulfonate (HPTS or pyranine).² The emission intensity (protonated/deprotonated) ratio of HPTS follows an intricate pattern against the surfactant concentration displaying at least three transition points (T₁₋₃). The ratio starts to increase above an initial concentration (T₁), attaining a maximum at an intermediate concentration (T₂), and after that, decreases again before leveling off at a higher concentration (T₃). Fluorescence anisotropy measurements of the methoxy analog 8-methoxypyrene-1,3,6-trisulfonate (MPTS) further revealed that the most organized state is near the critical point T₂. Moreover, isothermal titration calorimetry (ITC) showed maximum enthalpy change at the same composition confirming optimum interaction. Finally, we show that the assemblies containing ultralow concentrations of both F127 and cationic surfactant can be a useful medium for synthesizing gold nano-triangles.



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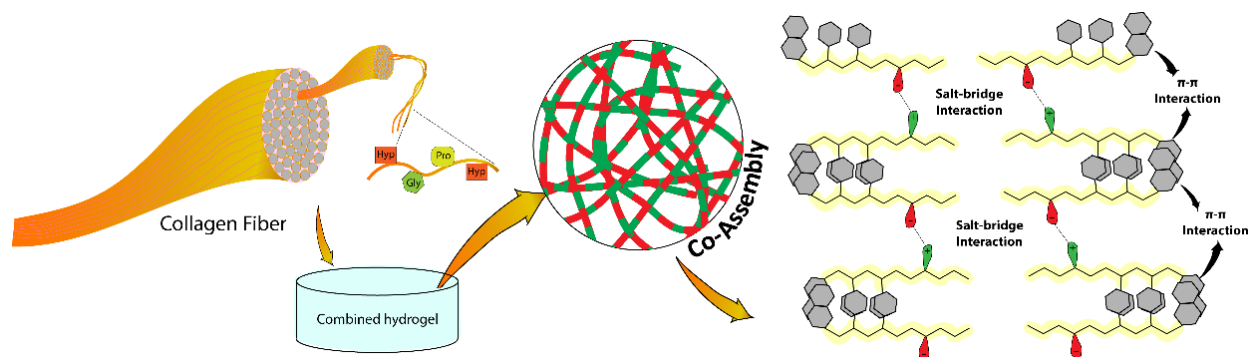
Developing Collagen Mimetic Ionic Complementary Peptide Hydrogels for Biomedical Applications

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The self-assembly of peptides and proteins into a well-ordered supramolecular structure is of great importance in physiology and pathophysiology. In our work, we aim to develop the biomimetic functional scaffold using self-assembling bioactive peptide sequences inspired from native extracellular matrix protein. In particular we have rationally designed two collagen mimetic peptides with the oppositely charged amino acids such as lysine and aspartic acid which can offer specific site for salt bridge interactions to induce the self-assembly within these peptides. Such coulombic interactions further trigger the formation of the self-assembled hydrogels at physiological pH. Very interestingly, a simple and facile strategy was utilized to maximize this attractive interaction by simply mixing the two components and switching the pH of the medium. From the spectroscopic and morphological studies, it was evident that peptides tend to form beta sheets and random coils at the nanoscale owing to their differential self-assembly. Furthermore, since the extracellular matrix composed of both peptides and carbohydrates, it is highly desirable to develop a conjugate matrix of peptides and sugars. Simple mixing of these bioactive peptides in carbohydrate matrix is expected to create an advanced synthetic extracellular scaffold with superior mechanical stability as well as biological properties. To this direction, we have explored the conjugate matrix of bio-molecular hydrogel based on cellulose, attached non-covalently to the short collagen mimetic peptides. Interestingly, these nano-porous structures within cellulose showed a great potential in tissue engineering and delivery matrices. Our current work is further focused on investigating the cell interaction behaviour with these designed peptide scaffolds and cellulose hydrogels for their applications in drug delivery, wound healing, and tissue engineering.

Keywords: Peptide self-assembly, collagen mimetic peptides, nanofibrous cellulose, electrostatic interaction.



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Self-Assembly and Micellar Transition in the Cationic Surfactant Triggered by the Alcohol

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This work reports the self-assembly and micellization behaviour of cationic surfactant in water and mixed alcohol-water solutions was investigated using various physicochemical techniques such as phase behavior study, tensiometry, conductivity, rheology, and small-angle neutron scattering (SANS) techniques. Here, three C_{16} -type cationic surfactant viz. N, N' -dihexadecyl- N, N, N', N' -tetramethyl- N, N' -ethanediy-diammonium dibromide (16-2-16) cetylpyridinium bromide (CPB), and cetyltrimethylammonium bromide (CTAB) were studied in presence of ethanol (co-solvent) 1-butanol (BuOH, mediator) and 1-octanol (C_8OH , co-surfactant) respectively. The studies suggested that the micellization process of 16-2-16 becomes delay and less spontaneous in the presence of ethanol because of ethanol locate within the aqueous bulk phase. Whereas, BuOH is promotes the mixed micelle formation of CPB micelle. In addition, the incorporation of C_8OH leads to an elongation of the ellipsoidal CTAB micelles. With the further addition of C_8OH , a transition of the elongated micelles occurred to a viscoelastic fluid comprising entangled wormlike micelles due to the solubilization of C_8OH within the CTAB micelle. These results will facilitate the optimization of processes and other comparable surfactants are used as phase transfer catalysts, structure-directing agents, or stabilizers in colloidal dispersions or emulsions.

Keywords: cationic micelles; alcohols; micellization; small angle neutron scattering (SANS).

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