



Prof. Sutapa Roy Ramanan

Senior Professor

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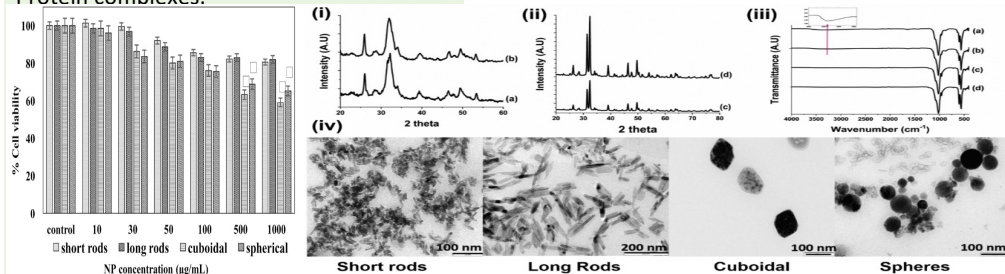
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There is plenty of room at the bottom.... - Richard Feynman

Areas of Interest: Nanomaterials, synthesis, application; Nanobiotechnology; Nanomaterials for corrosion protection, electrospun polymeric nanomotors

For in vivo applications, nanoparticles (NPs) are exposed to a range of biomolecules (majorly proteins) which forms a corona around the NPs (usually termed as protein corona (PC)), that significantly changes the surface properties of the NPs. This interaction between the NP and the protein may induce conformational changes in the latter contributing to various biological effects. Although NPs are being used for diagnosis and treatments, a complete understanding of the influence of various NP parameters on the function of the biomolecules is important. Our current research reports the synthesis of biocompatible hydroxyapatite (HAp) NPs of various morphology. These HAp NPs were surface functionalized with cetyl pyridinium chloride (CPC), having Cl⁻ as counter-ion, and their interaction with Pepsin A was studied to understand the role of the NP morphology on the NP-Protein complexes.



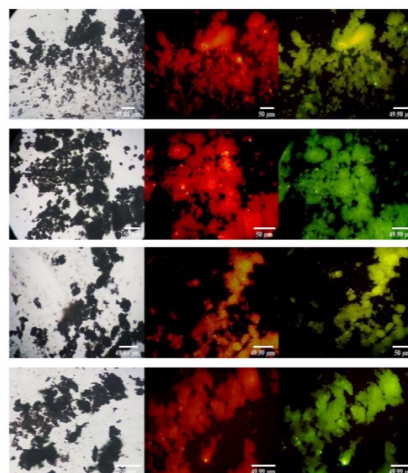
In recent years, hydroxyapatite (Ca₁₀(PO₄)₆(OH)₂, HAp) has garnered increasing interest in medicine because of its biocompatibility, bioactivity, and biodegradability, attributed to its compositional resemblance to the inorganic component of human bone and teeth. Structurally, nano-sized HAp (HAp NPs) possesses hexagonal crystal lattice where the calcium ions can be easily substituted by other divalent and trivalent ions without affecting its structural integrity. Applications of Ln doped HAp NPs in bioimaging and drug delivery are being explored. In our research, we report fluorescent Eu³⁺ and Sm³⁺ doped HAp NPs as bioimaging agents. A significant increase in the intensity has been achieved due to the self-activated fluorescent nature of the host HAp lattice.

Sponsored Projects: 10 (7 as PI & 3 as Co-PI); DRDO, DST, IRPA, INTEL, DBT Builder

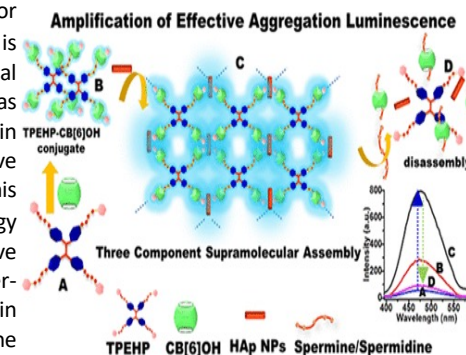
Ph.D. Guidance: 8 (completed 5; ongoing 3)

Publications: Patents-2; Journal-52; Conference-42

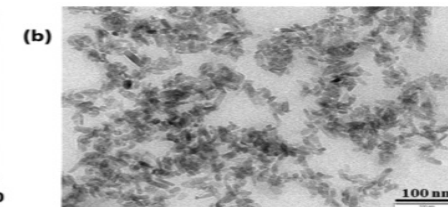
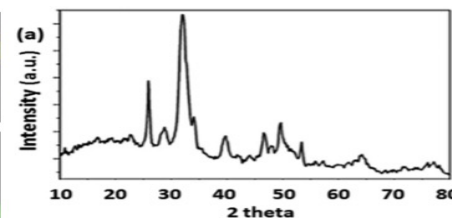
Google scholar Citation- 1817; **h-index-**18; **1-10index-**21



The development of sensitive and selective tools for the detection and quantification of biomarkers is important in the diagnosis and treatment of clinical diseases. Spermine (SP) and spermidine (SPD) act as biomarkers for early-stage diagnosis of cancer in humans as their increased levels in urine are indicative of abnormal biological processes associated with this fatal disease. In our research, we introduced a strategy for solid-supported amplification of the effective aggregation-induced-emission (AIE) effect of a water-soluble tetraphenylethylene (TPE)-based probe in developing a supramolecular sensing platform for the rapid, sensitive, and selective detection of SP and SPD in water. The sensing system showed low limits of detection (LODs) of 1.4×10^{-8} and 3.6×10^{-8} M for SP and SPD, respectively, which are well below the required range for the early diagnosis of cancer. Besides, a good linear relationship was obtained for both SP and SPD. Nominal interference from various



metal ions, anions, common chemicals, amino acids, and other biogenic amines makes this sensing platform suitable for the real-time, low-level measurement of spermine (and spermidine) in human urinary and blood samples.



Selected Publications:

- Effect of doping and surface functionalization on the conformational changes of protein upon interaction with hydroxyapatite nanoparticles", © 2020 Taylor & Francis Group, London, ISBN 978-0-367-43161-7, p3.
- Solid supported amplification of aggregation Emission: a tetra phenyl ethylene-cucurbit [6]uril@hydroxyapatite based supramolecular sensing assembly for detection of spermin in human urine and blood", ACS Applied Biomaterials.
- Design of a Biocompatible Hydroxyapatite-Based Nanovehicle for Efficient Delivery of Small Interference Ribonucleic Acid into Mouse Embryonic Stem Cells", MolecularPharmaceutics.
- Does the nanoparticle morphology influence interaction with protein:A case study with hydroxyapatite nanoparticle", materials Today Communications,



Prof. Srinivas Krishnaswamy

Professor

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“ Our main focus of research is in the area of Process Engineering and Intensification which involves addressing challenges posed in developing practical cost effective, energy efficient and environment friendly systems from a commercialization point of view, thereby attempting to bridge the gap between know-why and know-how.”

Research Interests: Process Engineering including synthesis, evaluation and intensification with emphasis on Unmixed combustion and its applications, gas hydrates, water treatment technologies for recovery & reuse, carbon di-oxide capture and other environmental friendly technologies

Patents: 4 Patents filed (2 granted)

PhD student guidance: 11 (5 completed, 6 ongoing)

Higher Degree (PG) Dissertations supervised: 10

Projects: 11 (9 funded / 2 non-funded)

Projects Ongoing: 2

Projects completed: 9

Project Funding till date: Sanctioned (~Rs. 8.41 crores), Received (~Rs. 8.45 crores)

Research Publications (Journals + Conferences): 18 (when in BITS Pilani) & 3 (before joining BITS Pilani)

Conferences presentations / Invited talks: 21 / 4

Teaching Interests: Chemical Engineering Thermodynamics; Kinetics and Reactor design, Process and Product Design Principles (synthesis, evaluation and economics)

Course taught till date: First Degree (UG): 15 and Higher Degree (PG): 6

First Degree projects supervised till date: ~120

Select administrative assignments undertaken in BITS Pilani: Group Leader and Head of Department (Chemical Engineering), Dean (Academic Graduate Studies, University-wide), Prof. in-Charge (CIIE, University-wide), In-Charge (CSIF), In-Charge (Student Sports activities), Warden

Selected Publications / Granted Patents

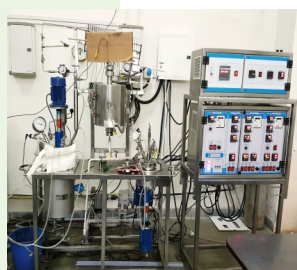
- **Srinivas Krishnaswamy**, Amol Deshpande & K. N. Ponnani, Chemical Engineering Science, 178, (2018), 367 – 376
- Parul Sahu, **Srinivas Krishnaswamy**, K. N. Ponnani & N. K. Pande, Desalination, 436, (2018), 144 – 151
- Parul Sahu, **Srinivas Krishnaswamy** & Nawal Kishore Pande, Chemical Engineering and Processing–Process Intensification, 153, (2020)
- Claire M. Welling, Siva Varigala, **Srinivas Krishnaswamy** and others, Science of the Total Environment, 730, 2020
- **Srinivas Krishnaswamy** et al., IN Patent 369080 (Granted), 2021
- **Srinivas Krishnaswamy** et al., IN Patent 419254 (Granted), 2023

The key focus of my research is in the area of Process Engineering & Intensification. The overall aim of my research is to overcome limitations imposed by thermodynamics and kinetics with regard to scale-up of process technologies, eventually leading to synthesis and development of practically feasible, energy efficient, environment friendly, safe and cost effective processes. In this regard, we have received funds to tune of approximately Rs. 8.5 crores from funding agencies like Ministry of Chemicals and Fertilizers, DST – SERB, Centre for High Technology (CHT), GAIL (India) Ltd. and Aditya Birla Group. I have worked on diverse applications from developing process schemes for treating process condensate water in fertilizer plants to investigating the role of electrochemical reactors for blackwater treatment. We hold granted patents related to a process scheme integrating LNG regasification with desalination and development of an environmental friendly process for co-chlorination of polyolefins. We are also the first in India to experimentally demonstrate a novel variant of combustion, i.e. “Unmixed Combustion” for 3 different applications (heat transfer, hydrogen production and CO to CO₂ conversion). We have recently ventured into researching the application of Machine Learning to Chemical Engineering systems. Several facilities have been created through the extra mural grants received:

- Unmixed Combustion/reforming, crude oil fouling and gas-liquid equilibrium test rigs
- Low temperature DSC; Gas hydrate autoclave
- Gas Chromatograph, HPLC, Atomic absorption and uV-spectrophotometer
- Multi-parameter water test kit; flat sheet membrane test rig



Unmixed Reforming Rig



Fouling test rig



High P, Low T DSC



Prof. S D Manjare

Professor

Dept of Chemical Engineering

!! WASTE TO WEALTH AND HEALTH !!

!! "To take along every single individual on common platform and form a responsible human chain to serve in the direction to humanity to achieve the target of "Sustainable Development" !!

Areas of Interest:

Process Systems Engineering, recovery of resources from waste streams/materials, development of new filler materials, environment management systems



- Process development to synthesize new grades of reinforcing materials to substitute the conventionally used fillers in elastomer compounds.
- Novel surface modification methods are being developed to enhance the adsorption of metal complexes on organic substrate. The new material has potential to use in polymeric matrix as fillers.
- Development of new methods, for recovery of valuable resources from waste materials, to be used, as an alternative to conventionally used fossil fuel based materials.
- Development of low cost and biodegradable biomass based filler materials / bio-adsorbents to be used as reinforcing fillers in polymer industry, treatment of wastewater streams, and drug delivery materials in pharmaceutical industry.
- Studies on modelling and simulations of various processes and heat exchanger network and wastewater treatment processes

Latest Publications

- "Recycling of waste tire by pyrolysis to recover carbon black: alternative & environment friendly reinforcing filler for natural rubber compounds" **Journal of Composite Part B: Engineering**, 200 (2020) 108346 (IF 9.078, H Index 146):.
- Experimental and theoretical investigation on pyrolysis of various sections of the waste tire and its components", **Chemical Engineering Research and Design** 179 (2022) 66–76 (IF. 4.119, H Index 108, SJR 0.79).



Prof. Saroj Sundar Baral

Professor

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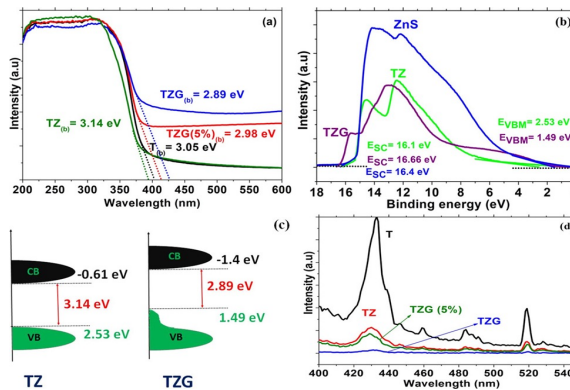
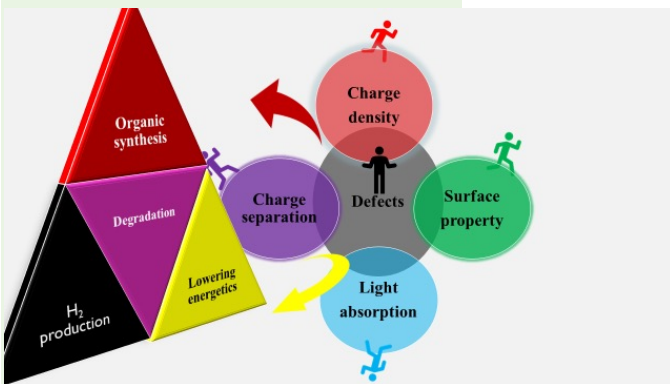
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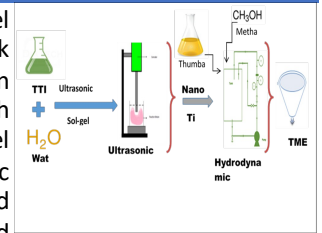
“Waste isn't waste until we waste it, Reuse the past, Recycle the present, Save the future”

Areas of Interest: Treatment & renewable resources recovery from wastewater using adsorption, anaerobic digestion and photo-catalytic degradation. chemical and biological extraction and purification of metals from ores and industrial wastes, Intensification different production processes for increase in quality parameter an reduce emission

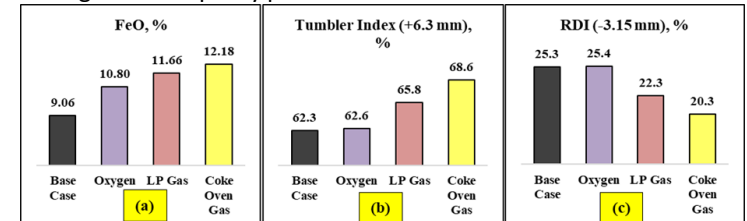
Developing an efficient photocatalyst for concurrent hydrogen production/CO₂ conversion and environmental remediation by using solar energy is a challenge. Although, defect engineering offers a strategical promise to enhance the photocatalytic performance, it has the limitations that come from the ambiguity surrounding its role. Our current research focusses on the comprehensive study of defects in promoting the charge transfer, band edge modulation, and surface reaction. Characterization techniques such as X-ray photoelectron spectroscopy, ultraviolet photoelectron spectroscopy, electron spin resonance, and photoluminescence are used to investigate defect functionality, and its ultimate effect on photocatalytic performance. In addition, efforts have been made to unveil the reaction pathway for hydrogen evolution reaction and oxygen evolution reaction where excess defect density greatly hampered the quantum yield of the process.



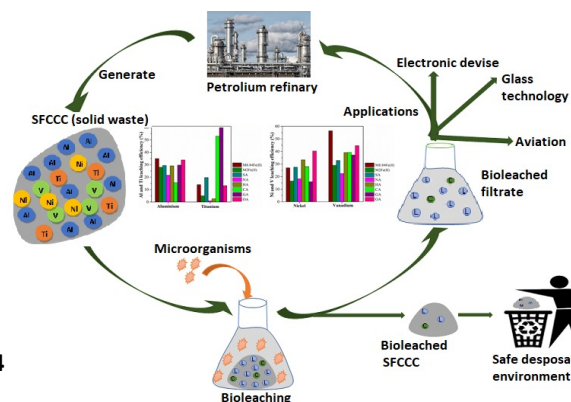
The development of clean and biofuel generation from sustainable feedstock using an integrated process intensification approach is essential. Current research focusses on intensifying biodiesel production process using hydrodynamic cavitation and heterogeneous catalyst and to find out the thermodynamics and kinetics of the biodiesel production.



The steel industry uses fossil fuel and therefore has a vital role in reducing the carbon footprint. The reduction of iron ore with gaseous fuels especially hydrogen is emerging as a promising field of research. In our current research, the effect of substituting the fossil fuel partly with gaseous fuels on CO₂ emission in sinter plants was assessed. The current research also aims at using the effects of recycling sinter waste gas on the quality parameters and emissions.



Industrial solid wastes are growing like a population due to rapid industrial outgrowth. The challenge in today's world is to manage these either by reuse or recycle to avoid landfilling. Hydrometallurgy and pyro metallurgy are the conventional techniques which are energy intensive and known to produce large pollutants. Bioleaching of metals from low-grade/industrial waste materials has evolved as an efficient and greener process. In our current research we intend to exploit the solubilization potential of different microorganism .



Sponsored Projects: 6 (3 as PI & 3 as Co-PI); DST, DBT & ABSTCPL
Ph.D. Guidance: 11 (completed 6; ongoing 5)
Publications: Books-2; Book Chapter-9; Journal-59; Conference-44
Google Scholar Citation- 2554; h-index-21; 1-10index-29

Selected Publications:

- Fundamentals and application of single atom photocatalyst in energy and environment sustainability, Renewable and Sustainable Energy Reviews, 167, (2022),112693
- Cleaner production of catalytic thumba methyl esters (Biodiesel) using TiO₂ nanoparticles under intensified hydrodynamic cavitation, Fuel, 313, (2022), 123021
- Defect engineering in photocatalysis: formation, chemistry, optoelectronics, and interface study, Journal of Material Chemistry A, 8(2020), 18560-18604.
- The effect of defects on optical, electronic and interface properties of NiO/SnO₂ heterostructures: Dual-functional solar photocatalytic H₂ production and RhB degradation, ACS Applied Materials and interface, 13, (2021), 60002-60017



Prof. Manjuri Kumar

Associate Professor

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Research Interest :

- Design, synthesis and characterization of novel copper and zinc complexes using different chelating ligands.
- Biological studies: DNA binding, DNA cleavage studies using metal complexes, protein interaction using Human serum albumin, cytotoxicity studies and anticancer activity of metal complexes on cancerous and noncancerous cell lines.
- Catalytic activity : investigation of catalytic activities of metal complexes such as Catecholase activity

Latest Publications:

Kumudini Paliwal, Paramita Haldar, P. K. Sudhadevi Antharjanam, and **Manjuri Kumar**: Mixed Ligand Mononuclear Copper(II) Complex as a Promising Anticancer Agent: Interaction Studies with DNA/HSA, Molecular Docking, and In Vitro Cytotoxicity Studies, **ACS Omega**, 7, 21961-21977 (2022).

Sidhali U. Parsekar, Kumudini Paliwal, Paramita Haldar, P.K. Sudhadevi Antharjanam, **Manjuri Kumar**: Synthesis, Characterization, Crystal Structure, DNA and HSA Interactions, and Anticancer Activity of a Mononuclear Cu (II) Complex with a Schiff Base Ligand Containing a Thiadiazoline Moiety. **ACS Omega**, 7, 2881-2896 (2022).



Prof. Sharad Sontakke

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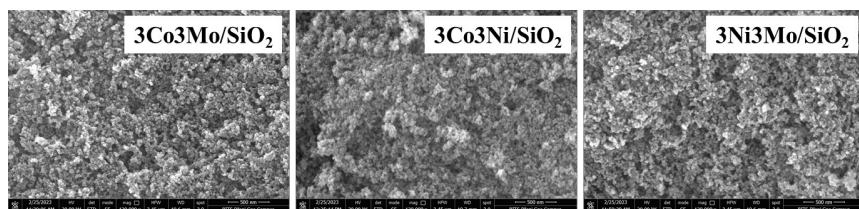
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In our research group we are working on synthesizing various catalysts and studying their applications for waste-water treatment, CO₂ capture, gas to liquid conversion, hydrogen generation, water splitting, etc. Our recent works are published in some of the popular international peer reviewed chemical engineering journals including Separation and Purification Technology, Advanced Powder Technology, Chemosphere, Chemical Engineering Journal Advances, etc. A glimpse of our research is presented below:

Catalysts for conversion of methane to higher hydrocarbon

Over the past century, the world's energy consumption has increased significantly due to an expanding population, industrialization and urbanization. Considering that fossil fuel reserves are depleting along with their impact on the environment, it is necessary to find an alternative low cost, abundant and environmentally benign source of energy. Natural gas has emerged as a key source of conventional energy due to improvements in excavation technology, incredibly low emissions as compared to other fossil fuels, and large reserves that are currently available in nature. The ongoing research work focuses on development of bimetallic catalysts on metal oxide supports for the direct non-oxidative conversion of methane.

We have developed a series of bi-metallic catalysts using combinations of Co, Ni and Mo doped on SiO₂, TiO₂ and Al₂O₃ support. Among the synthesized materials, Ni-Mo/SiO₂ displayed a maximum 11.5% initial methane conversion. The characterization of spent catalysts revealed no significant changes in the catalyst. The conversion of methane using bimetallic catalysts was superior compared to mono-metallic catalysts.



SEM image of synthesized catalysts

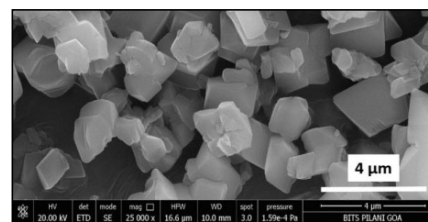
Areas of Interest: Metal organic frameworks, catalysis, wastewater treatment

Catalytic applications of Metal Organic Frameworks

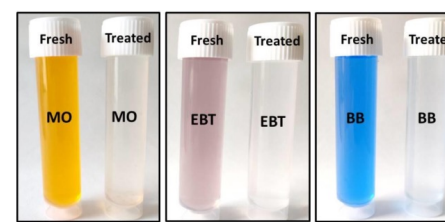
Synthesis of monometallic, bimetallic and trimetallic MOFs have been carried out. The thermal and water stability of the synthesized MOF have been tested. The synthesized materials were used for adsorptive removal of dye pollutants, photocatalytic degradation of organic pollutants, NaBH₄-mediated reduction of organic pollutants, etc.

The MIL-53 (Al) had a remarkable adsorption capacity towards anionic, cationic, or complex mixed dye solutions as well as real-time industrial effluent when used as an adsorbent. The material may be effectively reused up to many cycles. The results show that the nanocrystalline MIL-53 (Al) is very stable and recyclable, suggesting that it could be used in real applications.

When compared to pristine MWMIL and CS-TiO₂, the CS-TiO₂/MW-MIL composite material had a greater photoactivity.



SEM image of synthesized MOF



Images of fresh samples and treated sample for adsorption of dyes using MIL-53 (Al)

Latest Publications:

1. AA Meshram, SM Sontakke, 2022, Chemosphere 286, 131939 .
2. AA Meshram, SM Sontakke, 2021, Separation and Purification Technology 274, 119073.
3. AA Meshram, SM Sontakke, 2021, Advanced Powder Technology 32 (8), 3125-3135.
4. SD Parashar, SM Sontakke, 2023, Materials Today: Proceedings 72, 507-510.
5. SD Parashar, AA Meshram, SM Sontakke, Handbook of Nanomaterials for Wastewater Treatment, 833-846.

Google scholar: <https://scholar.google.com/citations?user=iYEhiVoAAAAJ&hl=en&oi=ao>



Prof. Vivek Rangarajan

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Research Specialization: Bioprocessing Engineering

Areas of Interest: Microbial products for applications in cosmetics, food, agriculture, pharmaceutical and environmental sectors. Green emulsion formulation and characterization for enhanced oil recovery, cosmetics and wastewater treatment applications, value addition of various agro-industrial wastes through bioprocessing methods

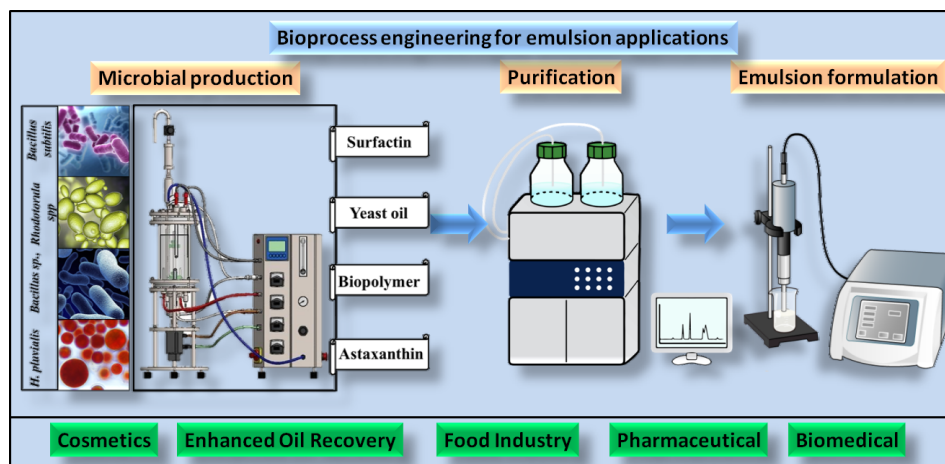
Biosurfactants for various applications: Biosurfactants are microbial-derived surfactants with superior properties such as high surface activity, low CMC, low toxicity and biodegradability. They are being increasingly researched for applications in agricultural, cosmetic, food, healthcare and oil recovery sectors. We have been focusing on the development of an intensified bioprocess for the concomitant production and purification of these surface active biomolecules in stirred tank fermentors. We developed a simple method for the synthesis of highly stable Ag-nanoparticles suspension, capped with lipopeptides, which showed very good antimicrobial properties. We have also developed a stable bio-cosmetic nanoemulsion with surfactin as green emulsifier, which remained stable for over a period of 6 months. Currently, we are working on other facades of these biosurfactants applications, such as in cosmetic formulations, antimicrobial and oil recovery.

Value added products from cashew plant:

Fermentation of cashew apple juice is still practiced as an art and hence systematic scientific understanding about Feni production as a whole in terms of process consistency, olfactory property and chemical quality parameters of the distillate will help improve commercial value of Feni product. It has been observed that some of Feni makers have shown interests in upgrading their production value, due to recent trend in increased foreign export. Thus, considering the growing need for upgradation of the existing feni making units possessed by cluster of small scale cashew producers and also owing to scarce reports on Feni production process in general, we aim to investigate the influence of these listed out factors on the overall quality of feni.

Biopolymers for various applications

We mainly focus on thermophilic bacteria for the production of thermo-tolerant biopolymers which have imminent potential for applications in food, cosmetics, fly-ash disposal, enhanced oil recovery etc. We exploring the feasibility of using various agro-industrial wastes as substrates for the production of bio-polymer through solar powered bioreactors.



Selected Publications

- Neela Gayathri Ganesan and Vivek Rangarajan. A kinetics study on surfactin production from *Bacillus subtilis* MTCC 2415 for application in green cosmetics. *Biocatalysis and Agricultural Biotechnology*. 33 (2021)
- Utkarsh Tiwari, Neela Gayathri Ganesan, Jui Junnakar & Vivek Rangarajan. Towards the formulation of bio-cosmetic nanoemulsions: From plant-derived to microbial-derived ingredients. *Journal of Dispersion Science and Technology* (2020).
- Divya J Mathias, Sourav Kumar, Vivek Rangarajan. An investigation on citrus peel as the lignocellulosic feedstock for optimal reducing sugar synthesis with an additional scope for the production of hydrolytic enzymes from the aqueous extract waste. *Biocatalysis and Agricultural Biotechnology*, 20 (2019) 1-8
- Vivek Rangarajan and Mahesh Narayanan. Biosurfactants in Soil Bioremediation. *Advances in Soil Microbiology: Recent Trends and Future Prospects*. Springer (2018).

Hydrolytic enzymes for the production of reducing sugars:

In years to come, the usage of ethanol-blended gasoline will become mandatory in all countries, as a measure to reduce the greenhouse gas emissions. So far, starch based feed stocks such as corn, sugarcane, potato and cassava have been used most widely for bioethanol production, but the motive of their use has led to the ever continuing debate of food vs fuel. Bioethanol production from lignocellulosic biomass has undoubtedly become a viable alternative, thanks to the improved biomass hydrolysis procedures through thermo-chemical methods. But, the focus in recent years has gradually been shifting towards the use of much cleaner and less-energy intensive process, such as, enzymatic processes for the hydrolysis of complex cellulosic substrates. To a greater extent, the research focus has been on lignocellulosic biomass from wood, grass and agricultural residues. Our current research endeavors are towards the use of fruit wastes from fruit processing industries as feed stock for the production of bioethanol. Also, we have been working on the production of biopolymers from the soluble sugars extracted from fruit wastes.



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Learn, Unlearn and Relearn

Areas of Interest: Water-Energy Nexus; Translational Research; Thermodynamics

The key focus of our group is to develop tangible solutions from understanding fundamentals of various technologies as well as developing new technologies.

We work on hydrodynamic cavitation, membrane separation, ozonation and apply tools like artificial intelligence, machine learning, Computational Fluid Dynamics and develop other mathematical approaches to understand the optimize these technologies at the benchscale. Then we try to develop workable prototypes to demonstrate the feasibility of the solution and understand feasibility of scale up and manufacturability.



Translational Research

We work on developing fundamental understanding of technologies and work on the economics and manufacturability as well as scale up of these technologies to bench top prototypes for field testing

Thermodynamics

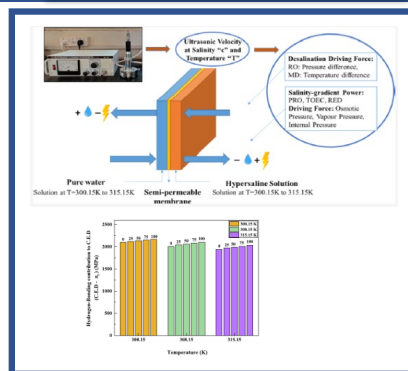
Our group works on determining thermodynamic properties of Salt-Water systems. This has tremendous applications in sectors like Oil and Gas (hydrofracking), Desalination and Blue Energy. We develop detailed understanding of Salt-Water interactions and develop engineering correlations for utilization in designing processes.

Latest Publications:

1. Anupam Mukherjee, Srinath Chalicheemala, Subhankar Roy, Aditi Mullick, Sirshendu De, Anirban Roy, and Siddhartha Moulik. "Design, development and performance evaluation of skid-mounted pilot wastewater treatment and resource recovery unit for mechanical scavenging vehicle." *Journal of Cleaner Production* 371 (2022): 133564. (IF : 11.072)
2. Rath, Rudra, Deepshika Dutta, Reddi Kamesh*, Mostafa H. Sharqawy, Siddhartha Moulik, and Anirban Roy*. "Rational design of high power density "Blue Energy Harvester" pressure retarded osmosis (PRO) membranes using artificial intelligence-based modeling and optimization." *Energy Conversion and Management* 253 (2022): 115160. (IF : 11.533)
3. Anupam Mukherjee, Aravind Satish, Aditi Mullick, Jyotsna Rapolu, Siddhartha Moulik*, Anirban Roy*, and Asim K. Ghosh*. "Paradigm Shift toward Developing a Zero Liquid Discharge Strategy for Dye-Contaminated Water Streams: A Green and Sustainable Approach Using Hydrodynamic Cavitation and Vacuum Membrane Distillation." *ACS Sustainable Chemistry & Engineering* 9, no. 19 (2021): 6707-6719. (IF : 9.224)
4. Anupam Mukherjee, Aditi Mullick, Siddhartha Moulik*, and Anirban Roy*. "Oxidative degradation of emerging micropollutants induced by rotational hydrodynamic cavitating device: A case study with ciprofloxacin." *Journal of Environmental Chemical Engineering* 9, no. 4 (2021): 105652. (IF : 7.968)

Water-Energy Nexus:

Our group works on problems related to the connection between energy and water and develop solutions (technologies and processes) keeping in consideration the holistic perspective. The group has expertise in membranes, hydrodynamic cavitation, ozonation, adsorption. We try to develop energy efficient technologies and benchmark against thermodynamic minimum energy to improve process design for Zero Liquid Discharge, Desalination and Salinity Gradient Power generation.





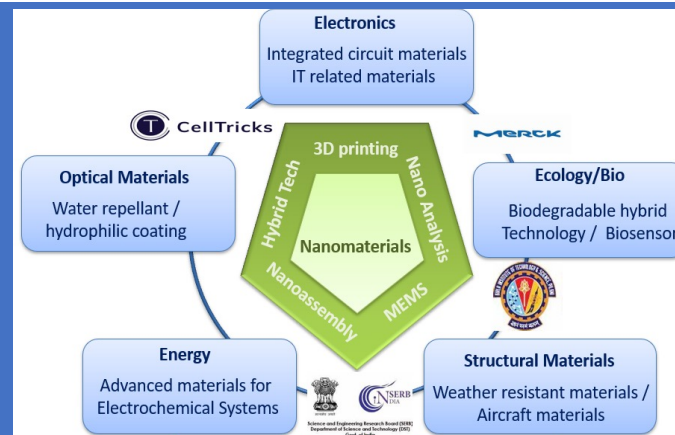
Prof. Jegatha Nambi Krishnan

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Areas of Interest: **Bio-MEMS – Microfluidic separation and detection technologies, Nanomaterials for sensor applications.**

Research Group Project highlights:

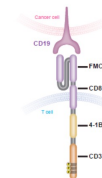
1. V. Kaarthick Raaja - Synthesis, Characterization and Investigation of Nano enhanced Blend membranes for desalination applications. Project focuses study on different blend proportions of sulfonated polybenzimidazoles and sulfonated Poly (arylene ether sulfone) (SPAES). Enhancement of membrane properties by dispersing Titanium Dioxide (TiO₂) nanoparticles in pristine and blend membranes. Lastly, to evaluate the performance of the synthesized membranes for effective desalination. The project is financially supported from the Department of Science and Technology – Science and Engineering Research Board (DST-SERB), Govt. of India (DST-SERB ECR/2015/000014).



Achievements:

- Venkatachalam, Kaarthick Raaja, Sachin MB Gautham, and Jegatha Nambi Nambi Krishnan. "Desalination characteristics of new blend membranes based on sulfonated polybenzimidazole and sulfonated poly (arylene ether sulfone)." *Polymer Bulletin* (2022): 1-20.
- Venkatachalam, Kaarthick Raaja, Sachin MB Gautham, Achyuth Anegondi Nateri, and Jegatha Nambi Krishnan. "Nano-enhanced sulfonated poly (arylene ether sulfone) composite membranes and their characterization." *High Performance Polymers* 34, no. 10 (2022): 1193-1203.
- J. Nambi Krishnan*, V. Kaarthick Raaja, S. Gautham, S. Narang and S. Mehra, "Sulfonated PBI based blend membranes for Desalination", International Conference on Desalination (InDA 2018) Clean India Technologies, Role of Desalination and Swachh Bharat Mission, NIT Tiruchirappalli, India.
- J. Nambi Krishnan*, V. Kaarthick Raaja and S. Gautham, "Acid polymer rich acid-amphiphilic blend membranes and their properties", The 6th International Water Association Regional Membrane Technology Conference (IWA-RMTC 2018), The M. S. University of Baroda, Gujarat, India.
- J. Nambi Krishnan*, V. Kaarthick Raaja and S. Gautham, "Amphiphilic polymer rich amphiphilic-acid blend membranes and their properties", The 15th International Conference on Polymer Science and Technology (SPSI-MACRO-2018), Indian Institute of Science Education and Research (IISER), Pune, Maharashtra, India.
- Thin film blend membrane for desalination - **202111019401**.

2. Prasanna Gururaj Joshi- Identification, design, prototyping, fabrication and analytical methods development of Microfluidic based sensors for CAR-T cells applications. There are multiple microfluidic sensors but the applications for CAR-T are limited and not appropriate and hence a need to design an appropriate sensor and other "T" cells type like Gamma/Delta also being tested using the sensor developed. Objective is intending to put in place a good device design development of the sensor which eases the isolation of cells from sample solution. The project is funded by CellTricks Biotech Pvt Ltd, Bangalore and Merck Lifesciences India Pvt Ltd for associated Chemicals and Reagents support.



Achievements:

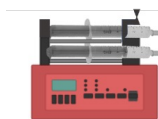
- Continuous flow microfluidic device for Enrichment of CAR T cells (**202111058598**).

3. Prathiksha P Prabhu - Identification, Separation and Detection of Microplastics from water samples. The primary focus of our study is to develop a hybrid automated technology where in the same device separation and detection can be carried out for MP present not only in natural water reservoirs but also in bottled water and various plastic packaged beverages. The project is being supported by the BITS Pilani, K K Birla, Goa campus.



Achievements:

- Prabhu, Prathiksha Prashanth, Koustav Pan, and Jegatha Nambi Krishnan. "MICROPLASTICS: Global occurrence, Impact, Characteristics & Sorting." *Frontiers in Marine Science* (2022): 1909.
- Patent (provisional application) title "Automated Continuous flow Microfluidic Device for the separation and detection of Microplastics in Water samples" (**202211068468**).



Others:

- Continuous flow microfluidic device for rapid heavy metal ion detection in water samples – **202011006180**
- Method for constructing large area synthesis of patterned complex metallic nanostructures and dissymmetrical tags – **202011006182**
- Electrochemical Microfluidic device for detection of heavy metal Ion in water samples - **202111017425**



Dr. Asima Shaukat

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Research interests:

- Rheological behavior of complex fluids like polymer nanocomposites, yield stress fluids, soft glassy materials
- Correlation of tribological performance and rheological behavior of lubricating greases
- Delayed yielding of particulate gels and nanocomposites

Predicting grease lubrication

Grease is extensively used as a lubricant in industrial rolling element bearings. The microstructure of grease is composed of a volume spanning network of thickener particles which are interlinked via weak van der Waals forces. The grease microstructure is highly sensitive to the applied stress, the duration of stress application and temperature. Consequently, grease rheological behavior is highly non-linear. For instance, grease viscosity may change by several orders of magnitude with variation in the applied conditions. Owing to the complex flow dynamics of grease, the lubrication mechanisms in grease lubricated contact are far from understood.

Our work focuses on developing correlations between grease microstructure, high shear rheology, and lubrication behavior. New methods for determining the grease flow behavior at extremely large shear rates are explored. The high shear rheology, determined from these methods, is used to estimate the grease film thickness inside the tribological contact. Moreover, we characterize the structural dynamics of grease in the quiescent-state and under flow through rheological measurements and microscopy. These results are compared with the lubrication performance of grease evaluated in terms of friction and wear.

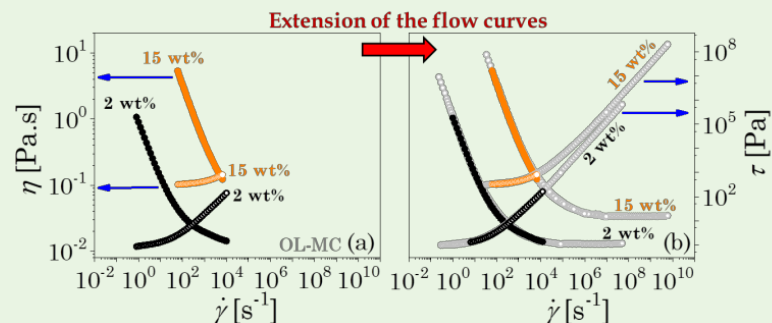


Fig. 1 Extrapolation of grease flow curves (shown in (a)) by employing τ vs. $\dot{\gamma}$ and η vs. $\dot{\gamma}$ master curves (gray curves in (b)) to tribological shear rates (10^6 to 10^7 s^{-1}).

Morphology, rheology and aging behavior of polymer nanocomposites

Clay-polymer nanocomposites find usage in a variety of applications as their mechanical, flame retardancy and gas barrier properties are substantially better than pristine polymers. When clay layers are added to polymer matrix, they form fractal clusters which interconnect to form a volume-spanning network of clay particles. The formation of this network greatly increases the elasticity of the material. However, inter-particle and particle-polymer thermodynamic interactions continuously work to change the dispersion of the clay particles in the polymer matrix. As a result, these materials undergo incessant morphological evolution with time. In this work, we systematically investigate the time-dependent changes in the microstructure of clay-polymer composites with the help of rheological measurements, X-ray diffraction analysis and electron microscopy over a period of several months. We analyze the results obtained from these three independent methods to gain insight into the morphological evolution of these materials with passage of time.

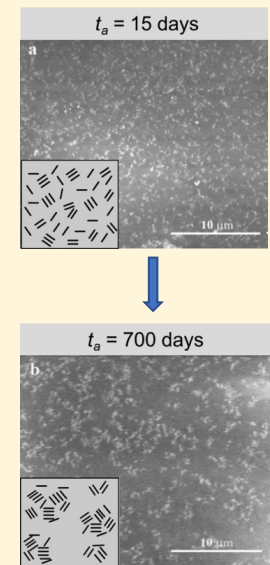


Fig. 2: Morphological evolution of PI/clay nanocomposite

Latest Publications:

1. Mubashshir, M., Shaukat, A. The Role of Grease Composition and Rheology in Elastohydrodynamic Lubrication. *Tribol Lett* **67**, 104 (2019). <https://doi.org/10.1007/s11249-019-1218-z>
2. Gavendra, A., Shaukat, A., Aging behavior of clay-polymer nanocomposites, 18th International Congress on rheology, Date: 2020/12/12-2020/12/17



Dr. Richa Singhal

Assistant Professor

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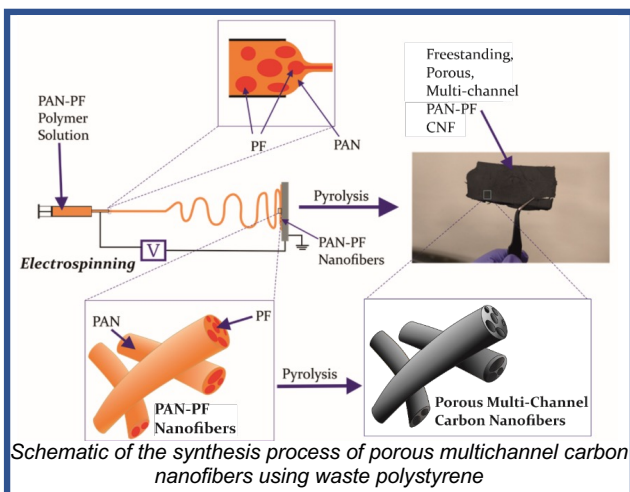
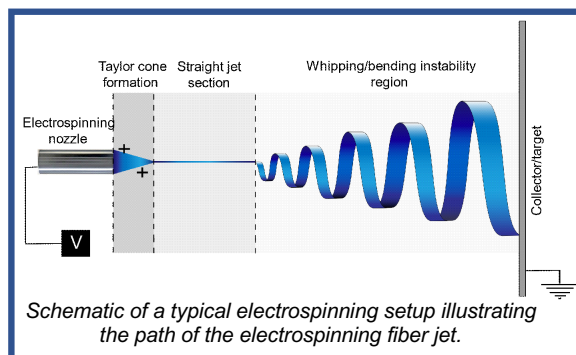
“The research group aims towards finding sustainable solutions to global energy issues. We currently work on developing low-cost and environmental-friendly nanomaterials and energy storage systems.”

Areas of Interest: Nanomaterials, Electrochemical energy storage, Supercapacitors, Rechargeable batteries

There are two major domains of my research: nanomaterials and electrochemical energy storage.

Nanomaterials

Our research revolves around developing effective and efficient nanomaterials with tuneable architectures, good stability and properties tailored for specific applications. We particularly synthesize electrospun nanofibers and their composites with metal oxides, MOFs etc that are versatile, free-standing, have high surface area, etc.



Electrochemical energy storage devices

We work on developing cost-effective and high-performance energy storage devices, particularly supercapacitors and batteries for portable electronics, electric vehicles as well as grid-energy storage. We aim to establish scalable technologies for the rapid-development of next-generation energy storage systems.

Modelling and simulation

We work on understanding the fundamentals involved in creating desirable surfaces and interfaces in order to design better materials for targeted applications.

Sponsored research projects:

- “Mechanistic approach to design composite metal-carbon nanofiber oxygen electrodes for high-performance metal-air batteries”, funded by **Early Career Research Award (ECR) – SERB-DST**, INR 45,59,920/-, 2018, PI: Richa Singhal, Co-PI, None.
- “Aqueous rechargeable metal-air batteries for large scale energy storage”, funded by **Additional Competitive Grant – BITS Pilani**, INR 8,77,000/-, 2018, PI: Richa Singhal, Co-PI, None.

Recent Publications:

- Radhakanth, S.; Singhal, R. In-situ synthesis of MnO dispersed carbon nanofibers as binder-free electrodes for high-performance supercapacitors. *Chemical Engineering Science*. **2023**, 265, 118224. I.F.: 4.889
- Sahoo, P.; Singhal, R.; Sow, P.K. Dynamic Electrolyte Spreading during Meniscus-Confined Electrodeposition and Electrodeposition of Copper for Surface Patterning. *ACS Applied Materials & Interfaces*. **2022**, 14, 37, 42586-42601. I.F.: 10.383
- Sow, P. K.; Singhal, R.; Sahoo, P.; Radhakanth, S. Fabricating low-cost, robust superhydrophobic coatings with re-entrant topology for self-cleaning, corrosion inhibition, and oil-water separation. *Journal of Colloid and Interface Science*. **2021**, 600, 358-372. I.F.: 9.965
- Gupta, A.; Ayithapu, P.; Singhal, R. Study of the electric field distribution of various electrospinning geometries and its effect on the resultant nanofibers using finite element simulation. *Chemical Engineering Science*. **2021**, 235, 116463. I.F.: 4.889
- Ishita; Singhal, R. Porous Multi-Channel Carbon Nanofiber Electrodes using Discarded Polystyrene Foam as Sacrificial Material for High-Performance Supercapacitors. *Journal of Applied Electrochemistry*. **2020**, 50, 809-820. I.F.: 2.925



Dr. Pradeep Kumar Sow

Assistant Professor

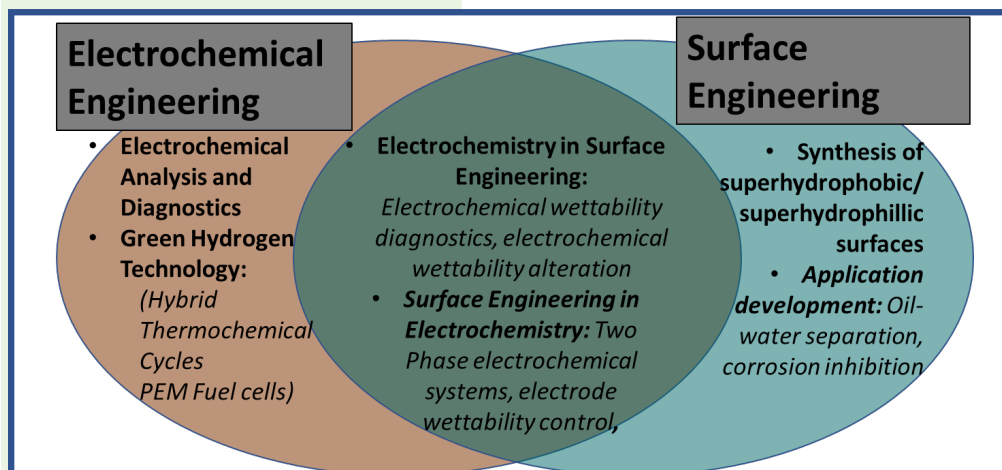
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Research with focus on developing novel solutions and applications by utilizing the fundamentals of Electrochemistry and Surface Science

Areas of Interest: Electrochemistry and Electrochemical Engineering, Surface Engineering and Interfacial Science, Hydrogen Technologies



Hydrogen Energy:

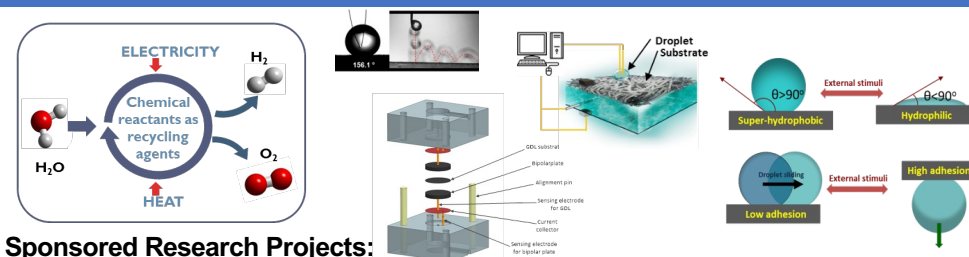
Increasing global warming has triggered an urgent need for the reduction of greenhouse gas emission and finding green energy alternatives. Hydrogen as an energy carrier is one of the most promising candidates to move towards realizing the green energy systems. Our research focuses on the development of economically viable and sustainable energy solution, with hydrogen as the energy carrier. Ongoing research is in developing efficient Thermochemical Cycles for Hydrogen production and Hydrogen Fuel Cell for electricity generation

Smart materials with an active control over the wettability:

Tuning the wetting behavior of a surface from hydrophobic to hydrophilic by inducing structural and chemical modifications is a innovative strategy for developing practical applications. In our lab we develop novel smart surfaces with electrochemically switchable wettability for on-demand wetting alteration. Along with material development we develop new applications using such smart materials

Diagnostic tools for understanding surface wettability:

In addition to the material and system development, we also strive to understand the wetting phenomenon by developing and using novel diagnostic tools and experimental approaches both on the surface as well as inside the porous structures.



Sponsored Research Projects:

- “Design Development and Bench Scale demonstration of electrochemical Hydroiodic Acid (HI) Decomposition in a Continuous Flow System for I-S cycle” study” funded by Oil and Natural Gas Corporation (ONGC) Energy Centre
- Continuous Flow Oil-Water Separation System Using Smart Separators Capable of Low-Voltage Wettability Switching”, funded by – SERB-DST,
- “Development of transition metal oxide based nanostructured surfaces for low-voltage tuning of wettability””, funded by Additional Competitive Grant – BITS Pilani,
- “Electrochemical Process for Hydroiodic acid (HI) decomposition in Iodine-Sulfur Cycle: A feasibility study ”funded by Oil and Natural Gas Corporation (ONGC) Energy Centre,

Selected Publications:

- Dynamic Electrolyte Spreading during Meniscus-Confined Electrodeposition and Electrodissolution of Copper for Surface Patterning. ACS Applied Materials & Interfaces. (2022), 14, 42586–42601
- Fabricating low-cost, robust superhydrophobic coatings with re-entrant topology for self-cleaning, corrosion inhibition, and oil-water separation. Journal of Colloid and Interface Science. (2021). 600, 358-372.
- Sustainable approach to recycle waste polystyrene to high-value submicron fibers using solution blow spinning and application towards oil-water separation. Journal of Environmental Chemical Engineering, (2020), 8, 102786
- A design framework for the fabrication of a low-cost goniometer apparatus for contact angle and surface tension measurements, Measurement Science and Technology, (2020),31: 125401



Dr. Amol Deshpande

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“The primary focus of all chemical industries is minimizing energy requirement and its effective utilization with least environmental impact. Our research group works on addressing these challenges and aims to develop cost effective and efficient alternative systems.”

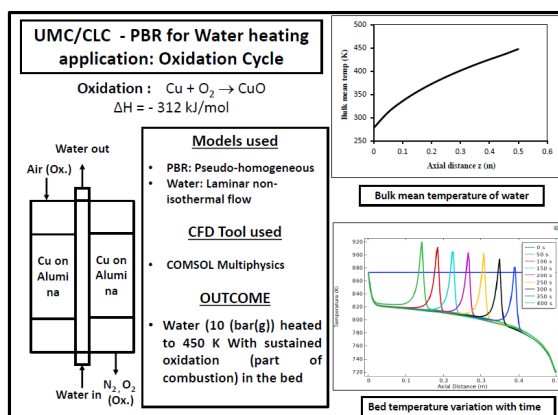
Areas of Interest: Chemical Looping Combustion / Unmixed Combustion, CFD, Process Intensification, Waste heat recovery, Multiphase flow in microchannels, Transport Phenomena,

In chemical industries, especially petroleum industries and in power plants, one of the primary objectives is to minimize energy demand, to effectively utilize and recover available energy and to reduce environmental impact. Although the research in the direction of using renewable energy sources looks a possible solution but its implementation in the existing industries has many practical limitations. Hence the main focus of our research group is to address these challenges by developing cost effective, energy efficient, environmentally friendly and sustainable alternative systems which can be implemented in the industries with relatively minor modifications. The research work involves experimental, modelling and CFD simulation studies of the proposed systems.

Unmixed combustion (UMC) for heat transfer applications

In industries, conventional combustion of fuel is used in steam boilers/furnaces that operate at high temperatures, are relatively bigger in size, and produce environmentally harmful NO_x and CO₂ mixed flue gases. These limitations can be addressed using an UMC process (a variant of chemical looping combustion (CLC)), an alternative to conventional combustion. In UMC, air and fuel are alternately passed over specific metal/metal oxides that undergo oxidation/reduction reactions and energy released can be used for relevant heat transfer applications.

- Proof of concept: Application of UMC for air heating - successfully demonstrated. (**Doctoral thesis**)
- Application of UMC/CLC for heating liquids like water (steam boiler system) and thermic fluids – ongoing (**BITS sponsored project**)
- Designing relatively effective monolith reactor systems for UMC/CLC applications – ongoing (**BITS sponsored project**)
- CO-fueled UMC application for power generation – ongoing (**DST Project – as a CoPI**)



CFD studies of fired boiler system

In the operation of fired tube boiler system, one of the important challenge faced is shrinking and swelling phenomena that occurs due to variation in steam demand in the plant. To address this issue, effective operation strategies need to be implemented. CFD studies of such system help in determining the desirable operating parameters based on the overall system behaviour, and are being carried out (**with Industry involvement**)

Waste heat recovery (WHR) in oil fired steam boilers

Conventional WHR systems in oil fired boilers have issues related to acid dew point corrosion that can occur due to reduction in flue gas temperature because of plant load variation. Hence the development of effective system (integration of heat pump with WHR system) to address this issue is being investigated (**with Industry involvement**).

Also, the research work in the specific areas of **Chemical Looping Water Splitting (CLWS) for hydrogen production, CLC for multiple effective evaporators and CFD study of multiphase flow micro-reactor (monolith) systems** have been initiated.

Latest Publications:

1. **S. Waikar, D. Jena, A. Deshpande***, A review on Chemical Looping Water Splitting (CLWS) as a potential alternative to Steam Methane Reforming (SMR) for hydrogen production, Journal of Physics: Conference Series (4th International symposium HEET 2021 – 19th to 20th Nov 2021 online), 2208 (2022) 012015.
2. **Amina Faizal, Amol Deshpande***, Modeling and CFD simulation of heat transfer process coupled with Unmixed Combustion for the application of generating superheated steam. Applied Thermal Engineering, 209 (2022) 118286
3. **Amol Deshpande, Amina Faizal**, Development of an unmixed combustion (UMC) based water heating system – Modeling and CFD simulation study for the oxidation cycle. Thermal Science and Engineering Progress 24 (2021) 100924.
4. **Amol Deshpande, Aastha Arya**, Comparative CFD simulation studies on monolith and packed bed reactors for oxidation of Cu in unmixed combustion (UMC) process. **Chemical Engineering Research and Design** 160 (2020) 521–532.
5. P. Sai Pavan Kalyan, **Amol Deshpande***, CFD Simulation of Fuel/flue gas section of the fire-tube steam boiler system, Proceedings of the 6th World Congress on Mechanical, Chemical, and Material Engineering (**MCM'20**) [7th International conference HTFF'20], Virtual Conference August 16 – 18, 2020
6. **Amol Deshpande, Srinivas Krishnaswamy, Krishnaswamy Ponnani**, Experimental investigations on unmixed combustion for heat transfer applications. **Chemical Engineering Science** 164 (2017) 122 – 132.



Dr. Paramita Halder

Assistant Professor

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“ All of us hold the potential to revolutionize how we remedy the non-renewable environment around us. Our research group focuses on problems related to the energy storage, drug delivery and we are looking for solution for preservation of heritage monument. ”

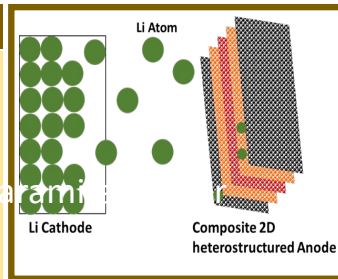
Areas of Interest: Molecular Modeling, Protein Docking, Drug delivery and Energy Storage materials, Electronic Properties Calculations (Density Functional Theory), Molecular Dynamics Simulations, Finite Element Method Analysis

Molecular modeling is required to understand the kinetic mechanism, binding affinity, electronic properties and structural evaluation of energy storage materials, bio-molecules.

A new direction of electrode materials towards next-generation energy storage devices

Objectives:

- Design of novel new two-dimensional (2D) Vander Waals heterostructured materials as electrodes in lithium ion battery
- Investigation of structural, electronic, adsorption and diffusion properties of newly developed 2D heterostructured material
- Model the Li atom and heterostructured anode materials to understand the solid-solid interaction, intercalation reaction mechanism

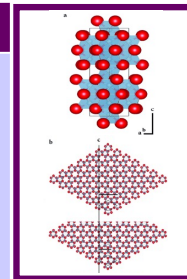


Dr. Paramita

Molecular Dynamics Simulation of Hybrid Nanofluid (HyNF)

Objectives:

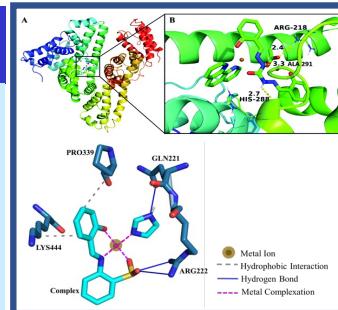
- Investigation of the stability of proposed HyNF
- MD Study of thermal behavior of HyNF under different environments
- Correlate physical and rheological attributes of selected HyNF with their stability
- Derive a correlation function representing the thermal behavior



Molecular docking and Molecular Dynamic studies to understand the binding affinity and structural evaluation of Human Serum albumin (HSA) with drug molecules

Objectives:

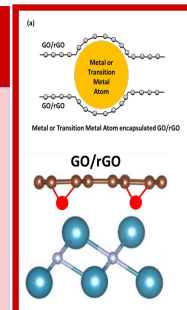
- Determination the kinetic mechanism underlying the Cu(II)/Zn complex-human serum albumin (HSA) interaction at the molecular level.
- Calculation of the free energy change, bioactivity, physicochemical properties and different thermodynamic parameters.
- Development of Artificial Intelligence based predictive computational models to predict the drug delivery and the encapsulation efficiency.



2 dimensional heterostructures on graphene oxide and reduced graphene oxide for molecular and atomic hydrogen storage

Objectives:

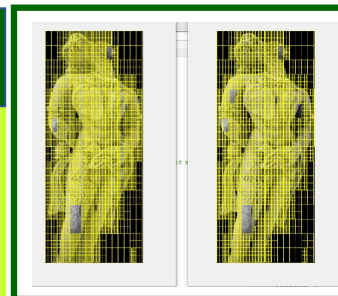
- Study the stability of the metal nanoparticles doped or encapsulated structures
- Calculate the electronic properties
- Study the Coulomb and Kubas interaction between molecular (H₂) and atomic (H) hydrogen
- Investigation of the adsorption energies



Computational and geotechnical studies on preservation of heritage monuments in the arid and semi-arid regions of Western India

Objectives:

- Characterization of the construction material of the monuments and evaluate its physical properties
- Investigation various impact of climate and biological effects on the materials of the monuments
- Fracture analysis using Finite Element Method



Latest Publications:

1. Halder et al. Dalton Transactions, Royal Society of Chemistry, 49: 2947-2965 (2020).
2. Halder et al, Applied Organometallic Chemistry, John Wiley & Sons, Ltd, DOI: 10.1002/aoc.6152 (2021; e6152).
3. Halder et al., ACS Omega, 7, 2881-2896 (2022).
4. Halder et al., ACS Omega, 7, 21961 – 21977 (2022).
5. Halder et al. Springer nature, (2023) (accepted).
6. Halder et al. Structural Geology and Tectonics Field Guidebook—Volume 2, Pages 359-418 (2023).



Dr. Sundari R

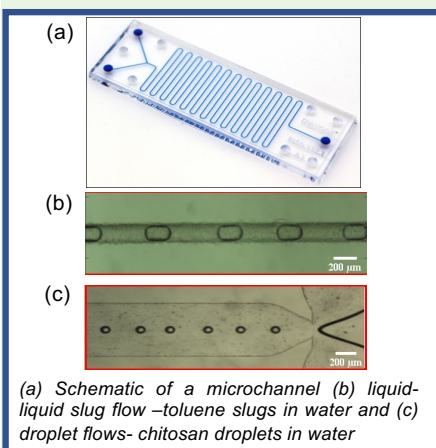
Assistant Professor

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My research interests primarily span two broad areas, viz., transport phenomena in multiphase flows and Systems Biology. With respect to the former, my focus has primarily been on developing semi-analytical mathematical models as well as computational fluid dynamics using the interface capturing level set method. In the field of systems biology, I am specifically interested in modelling cellular networks, integrating different biochemical processes in a cell, and disease modelling.



Numerical Investigation of Marangoni effects in liquid-liquid slug flows

This study aims at numerically studying Marangoni effects on liquid-liquid slug flow dynamics for two cases (i) an unbounded/unconfined domain and (ii) in microchannel. The main objective of this study is to understand how droplets behave with and without a surfactant and get conclusive results on how the presence of a surfactant affects mixing within the slug/droplet. Towards this, we develop an in-house mathematical model which can efficiently describe liquid-liquid slug flows for the two cases using the Level Set Method (LSM). Surfactant – laden droplet flows are modelled to analyze Marangoni convection and its effects on the hydrodynamics (vortex patterns, velocity, and pressure fields) and mixing intensity. The effect of confinement on Marangoni convection would be understood. This study would provide conditions which give rise to enhanced mixing in liquid-liquid slug flows.

Droplet coalescence

Controlled coalescence is an important means employed to initialize reactions between two droplets consisting of different reagents. The droplet pair approaches each other and coalesces to form a single droplet. In the process, the reagents present in the two droplets mix and react to form the desired product. Droplet coalescence can be induced by either active or passive methods. Droplet coalescence can be triggered by manipulating the physical properties of the two droplets. We focus on understanding the phenomenon of coalescence of droplets in the presence of a surfactant for different fluid properties using experiments and numerical simulations.

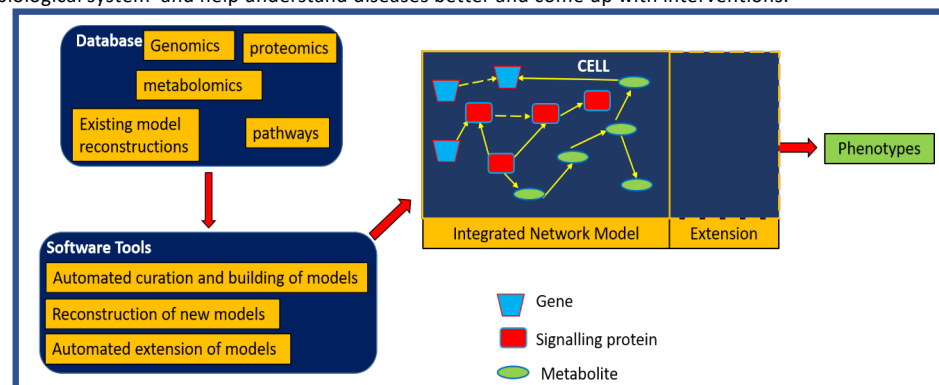
“ The important thing is to not stop questioning. Curiosity has its own reason for existing. - Albert Einstein

Our research focuses on studying both fundamental and application-oriented technologically relevant problems

“ Areas of Interest: Transport Phenomena, multiphase flows, microfluidics, Computational Fluid Dynamics, Systems Biology

Systems Biology

The functioning of a cell requires multiple processes to act in an integrated manner. The cross talk between the i) metabolic (ii) signaling and (iii) gene regulation networks lead to cellular phenotypes. With the advent of Systems Biology, the study of these networks has become a crucial tool for understanding the cellular processes and disease management. Mathematical models have been developed to analyze the metabolism, signaling and regulation in various life forms and have provided accurate description of cellular processes. Most of the models developed so far have analyzed metabolism, signaling and regulation in isolation, without considering the interactions between the different networks. This study aims at developing a generic mathematical framework to seamlessly integrate the signaling and metabolic networks in any biological system. The integrated model is expected to provide better insights of the biological system and help understand diseases better and come up with interventions.



Latest Publications:

- **Sundari Ramji**, Arjun Rakesh and S. Pushpavanam, *Modelling mass transfer in liquid-liquid slug flow in a microchannel*, Chemical Engineering Journal, Volume: 364, Pages: 280-291, 2019
- **Sundari Ramji** and S. Pushpavanam, *Liquid-liquid extraction in laminar two-phase stratified flows in capillary microchannels*, Chemical Engineering Science, Volume: 195, Pages: 242-249, 2019
- **Sundari Ramji**, Anil Vir and S. Pushpavanam, *Two phase gas-liquid stratified laminar flows in tubular reactors sustaining liquid phase reactions*, Chemical Engineering Journal, Volume: 356, Pages: 609-621, 2019



Dr. Riju De

Assistant Professor

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The key focus of our research is to develop advanced model-based control strategies for waste to energy conversion processes. Our research involves process systems engineering applied to various thermochemical processes such as hydrothermal pretreatment and hydrothermal liquefaction involving conversion of various lignocellulosic feedstocks to biofuels.

Batch Process Optimization and Control

Our primary focus is to optimize and control batch processes because they are highly non-linear, do not exhibit any steady state, and have a wide range of operating conditions. Therefore, conventional PI or PID controllers may fail to achieve satisfactory control of the set point profiles and hence, a model-based control approach becomes essential.

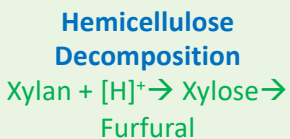
Pretreatment of Lignocellulosic Biomass

Lignocellulosic biomass (LB) is proven to be an excellent source of renewable energy because they avoid the food vs. fuel competency and can be successfully converted to ethanol or butanol via a biochemical processing route. Lignocellulose is composed of hemicellulose, cellulose, and lignin. Pretreatment is the first step in biomass conversion, which solubilizes the hemicellulose and lignin content from the biomass. Thus, cellulose becomes more accessible for the subsequent enzymatic hydrolysis to produce monomeric sugars, viz. xylose and glucose. These monomeric sugars can further be fermented to produce bioethanol or biobutanol.

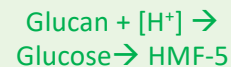
Major components of lignocellulosic biomass

- Hemicellulose - Xylan
- Cellulose - Glucan
- Lignin

HTP process reactions



Cellulose Decomposition

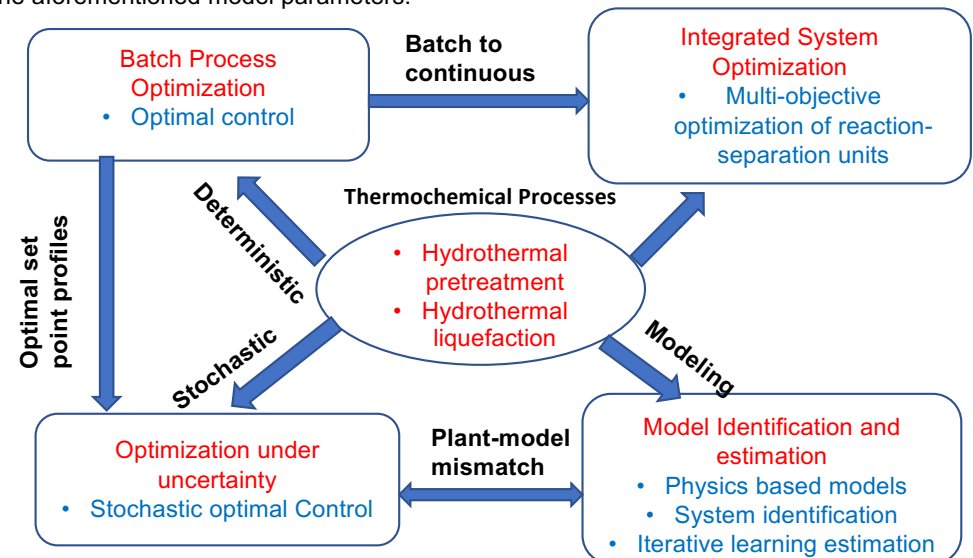


“ Whenever any real life uncertainties hit us in whatsoever manner, a process system’s engineer always has a weapon called stochastic optimization to respond to those uncertainties with brute force and in a robust manner ”

Areas of Interest: Optimal control, Multi-objective optimization, Batch-to-batch Iterative Learning Control, Stochastic Optimization

Hydrothermal Pretreatment (HTP)

Hydrothermal pretreatment (HTP) is a promising method used to disrupt the recalcitrance structure of LB using either hot water or steam, which is usually performed at a higher temperature ranging from 150-240 °C and pressure between 1-3.5 MPa. A higher temperature is beneficial to obtain maximum sugar yields. However, too high a temperature leads to degradation products, e.g., furfural and 5-hydroxymethylfural during the HTP step, which significantly inhibits the downstream fermentation. Moreover, the effect of other parameters such as choice of feedstock, amount of hot water or steam used, and reaction time play a vital role in influencing sugar yields. Therefore, a model-based optimization is essential to generate the maximum yield of sugars while optimizing the aforementioned model parameters.





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Research Exposure:

In PhD, I exclusively worked on the fabrication of functionalized polymeric nanofibers by encapsulating the therapeutic agents and active molecules, and studied their release and applicability in *-vitro*. In healthcare, three different problems are focused based on oral, transdermal and topical routes respectively, wherein the stability, solubility and toxicity of drug molecules such as Amphotericin B, Diclofenac Sodium and herbal drugs such as honey and curcumin, were tackled by applying different controlled release strategies. The similar principles were then employed in Agriculture where I worked on to address pre and post-harvest losses by introducing controlled release of fertilizer and by fabricating ideal seed storage bags.

Electrospinning is a fiber generation technique which utilizes electric force to draw micro/nano fibers from a conducting polymeric solution. The as fabricated nanofibers are endowed with some interesting features such as high surface to volume ratio, high porosity, interconnectivity and easy encapsulation of active molecules such as drugs. Till date various kinds of therapeutic agents have been encapsulated or immobilized or surface functionalized on polymeric nanofibers in order to preserve the bioactivity and therapeutic efficacy of the active molecules along with the desired release rate. For example, drugs having low half-life or shelf life such as NSAIDs, herbal extracts, essential oils or natural drugs are encapsulated to improve its stability.

The easily degradable active molecules such as vitamins, proteins, enzymes, DNA, RNA have also been loaded. For local/transdermal therapy such as wounds, burn, and tumor, the anti-oxidant, anti-microbial and anti-cancer agents are efficiently encapsulated in to the nanofibers and their applications have been tested *in-vitro/ in-vivo* with few undergone through clinical trials. This motivates me to define following key objectives focusing on natural drug loaded bio-polymeric nanofibers for drug delivery and tissue engineering.

Key objectives:

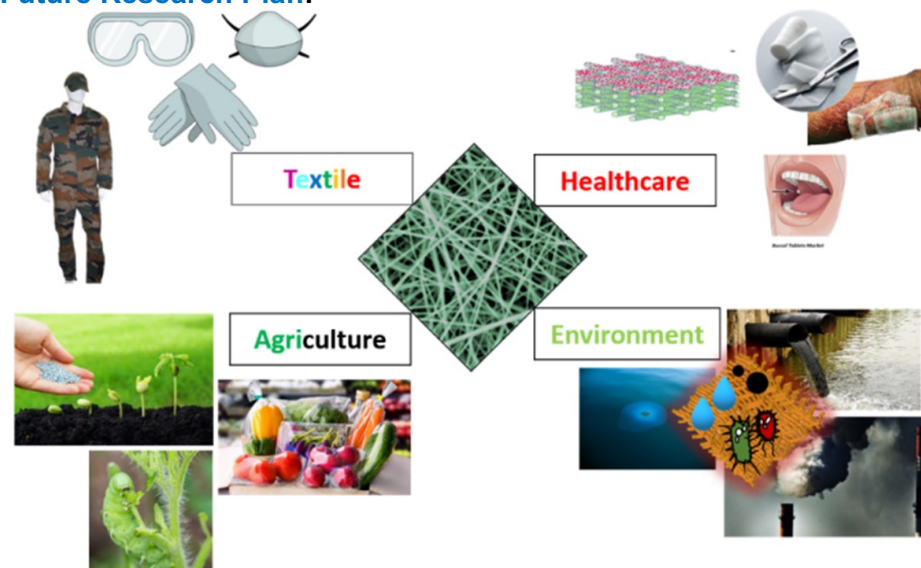
- 3 D patterned scaffold as an *in-vitro* cancer model
- Aligned and Randomly deposited nanofibers for bone tissue regeneration
- Transdermal patches / wound dressing mats for burn injury, muscular pain and post-surgical wounds.
- Buccal tablets for mouth ulcers

“ अत्त दीपो भव : Be your own light. ”

-Gautam Buddha

Areas of Interest: Functionalized Nanomaterials, Electrospun nanofibers, Compressed nanofibrous oral tablets, Controlled release of active molecules, Drug delivery, Pre- and post-harvest losses in agriculture, Controlled release fertilizers, Seed storage bags, environmental remediation

Future Research Plan:



List of Publications:

1. Gaydhane et al. *RSC Advances* 13(2023), 7312-7328.
2. Gaydhane et al. *Journal of applied polymer science* 138 (2021):50003.
3. Gaydhane et al. *Journal of Materials Research* 35(2020):600-609.
4. Gaydhane et al. *Materials Today Communications* 24 (2020): 100953.
5. Gaydhane et al. *Nano-structures & Nano-objects* 19 (2019): 100367.
6. Gaydhane et al. *Biomufacturing Reviews* (2018) 3:1.
7. Gaydhane et al. *Applied Surface Science* 426 (2017): 755-762.
8. Gaydhane et al. (2020). Jenny Stanford Publishing Pte Ltd, Singapore (2020) 507-542 (Book Chapter)



Dr. Upasana Mahanta

Assistant Professor

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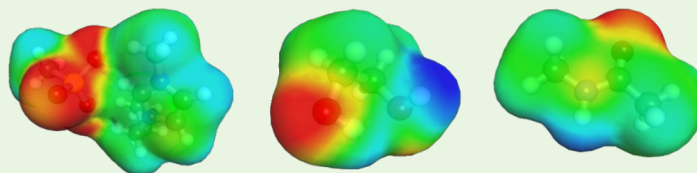
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My research interest primarily includes non-aqueous solvents for energy storage and environment. The majority of my work integrates experimental investigation and molecular dynamic studies of Ionic liquids, polymeric ionic liquids, eutectic mixtures for batteries and supercapacitors. I also have a keen interest in electrode materials for electrochemical energy storage.

Ionic Liquids (ILs)

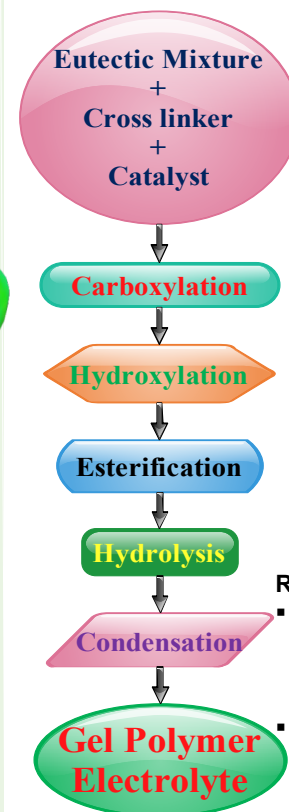
ILs are basically composed of ions: an organic cation and either organic or inorganic anion, having melting point lower than 100 °C. The flexibility in cation-anion combinations results in a wide variety. ILs are well known for their non-flammability, low volatility, thermal and chemical stability and hence they cover wide range of applications. Moreover, reasonable ionic conductivity and higher ESPW are the two more attractive properties of ILs or RTILs for their use in electrochemical storage device.



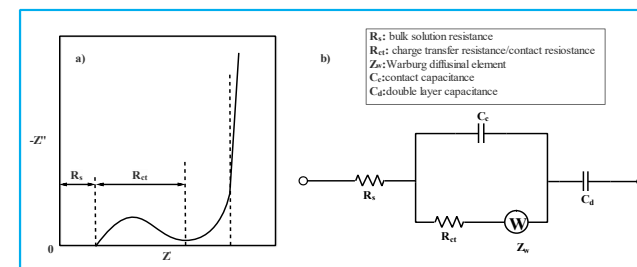
Polar and non-polar regions of Eutectic Solvents

Deep Eutectic Solvents (DES)

DESs constitute another class of newly emerging solvents, which is earning a lot of attention from the scientific and industrial community for their attractive physicochemical properties. A DES is a eutectic mixture of a hydrogen bond acceptor and a hydrogen bond donor which are associated through hydrogen bond interactions, when those are mixed in a specific molar ratio. The newly formed phase is characterized by a freezing point, which is lower than the fusion or melting temperatures of both the constituent materials. They possess similar physicochemical properties to ILs. The cost effectiveness of DESs over conventional ILs bring out their applications in different fields of chemical and electrochemical engineering.



Gel polymer electrolyte from Eutectic Solvents



a) Schematic of an impedance plot and b) equivalent electrical circuit for supercapacitor

During the period of advancements in electrochemical devices, energy and power densities are being considered as the two most important parameters. An electrochemical capacitor can deliver the stored energy in a faster rate than batteries whereas batteries can store more energy. To have energy density equivalent to batteries, an electrolyte with greater electrochemical stability is required for supercapacitor.

Recent Publications

- S. Choudhury, U. Mahanta, R. P. Venkatesh and T. Banerjee. Ionic Liquid Derived Novel Deep Eutectic Solvents as Low Viscous Electrolytes for energy Storage. *Journal of Molecular Liquids*. 2022, 366, 120245
- U. Mahanta, S. Choudhury, R. P. Venkatesh, S. Sarojiniamma, S. A. Ilangovan and T. Banerjee. Ionic-Liquid-Based Deep Eutectic Solvents as Novel Electrolytes for Supercapacitors: COSMO-SAC Predictions, Synthesis, and Characterization. *ACS Sustainable Chemistry and Engineering*. 2020, 8, 372-381



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Waste is failure of human imagination.
Nothing is waste and everything is a resource.
At the end of product life, everything needs to go
back to where it came from.

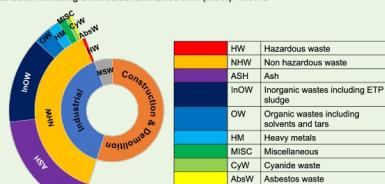
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Areas of Interest: Waste management and Valorisation, Green Chemistry and Technology, Catalysis

My research interest is in the area of waste management and valorization (or value addition), green chemistry and technology with focus on catalytic technologies. I investigate strategies for valorization of renewable and non-renewable industrial waste streams by adopting a systems approach such that the waste stream in each industrial operation is identified and processed at the point of generation.

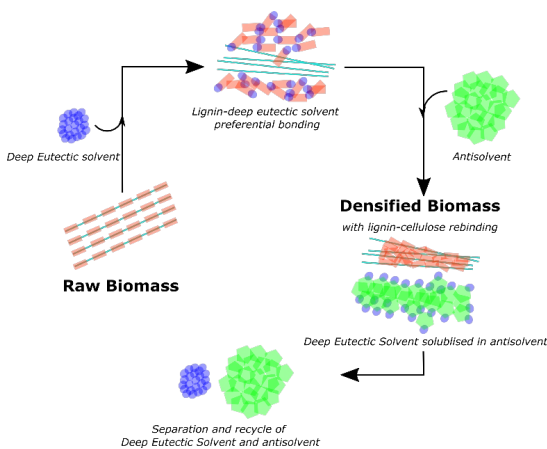
Waste tonnage in India

- Industrial : 39.45%
- Construction & Demolition : 54.87%
- Municipal Solid Incuding Biomedical and Electronic (MSW) : 5.67%



Densification of biomass waste

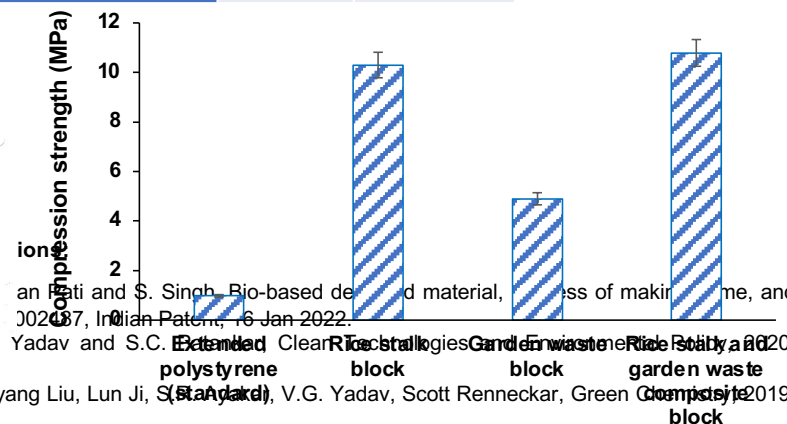
Agricultural and horticultural waste is a source of carbon, hydrogen and oxygen that must be harnessed effectively. The morphology of biomass can be altered by manipulating the hydrogen bonding between cellulose and lignin at atmospheric pressure and enabling formation of blocks/sheets/balls/pellets from any biomass samples consisting of loose particles. A deep eutectic solvent consisting of hydrogen bond donor and hydrogen bond acceptor is mixed with biomass sample. The lignin is separated from cellulose by the deep eutectic solvent in the reactor and then repolymerized with cellulose on addition of antisolvent thereby altering the hydrogen bonding between cellulose and lignin which gives unique morphology to biomass. The deep eutectic solvent is dissolved in added antisolvent and can be recycled.



Properties of densified biomass

The densified biomass samples exhibit higher energy density, higher compression strength and porosity that make them suitable for bioenergy, packaging and insulation applications.

Sample	GCV (Cal/g)	GCV (Cal/cm ³)
Raw biomass (typical)	3500	700
Rice stalk biomass block	3509	5319.6
Garden waste biomass block	4047	6515.7
Rice stalk + Garden waste (1:1) mixture biomass block	3949	5603.6



- Patankar, S. C., and S. Singh, Bio-based densified material, process of making same, and its application, Indian Patent, 16 Jan 2022.
- V.G. Yadav, G.D. Yadav and S.C. Patankar, Extended Clear Rice stalks, Garden waste, Rice stalk + garden waste composite, 2020, 22, 1757–1774.
- S.C. Patankar, Li-yang Liu, Lun Ji, S. Sankar, V.G. Yadav, Scott Rennecker, Green Chemistry, 2019, 21, 785-791.
- S.C. Patankar, Scott Rennecker, Green Chemistry, 2017, 19, 4792-4797.





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Research Specialization: Bioprocess Engineering

Areas of Interest: Biofuel (2G bioethanol, biodiesel, bio-crude) production from various low-cost substrates like lignocellulosic biomass, distillery or food processing wastewater. Developing sustainable biorefinery models, thermo-chemical processes for biofuel production, bioprocess optimization, life cycle assessment.

Biofuel production from lignocellulosic biomass (LCB) :

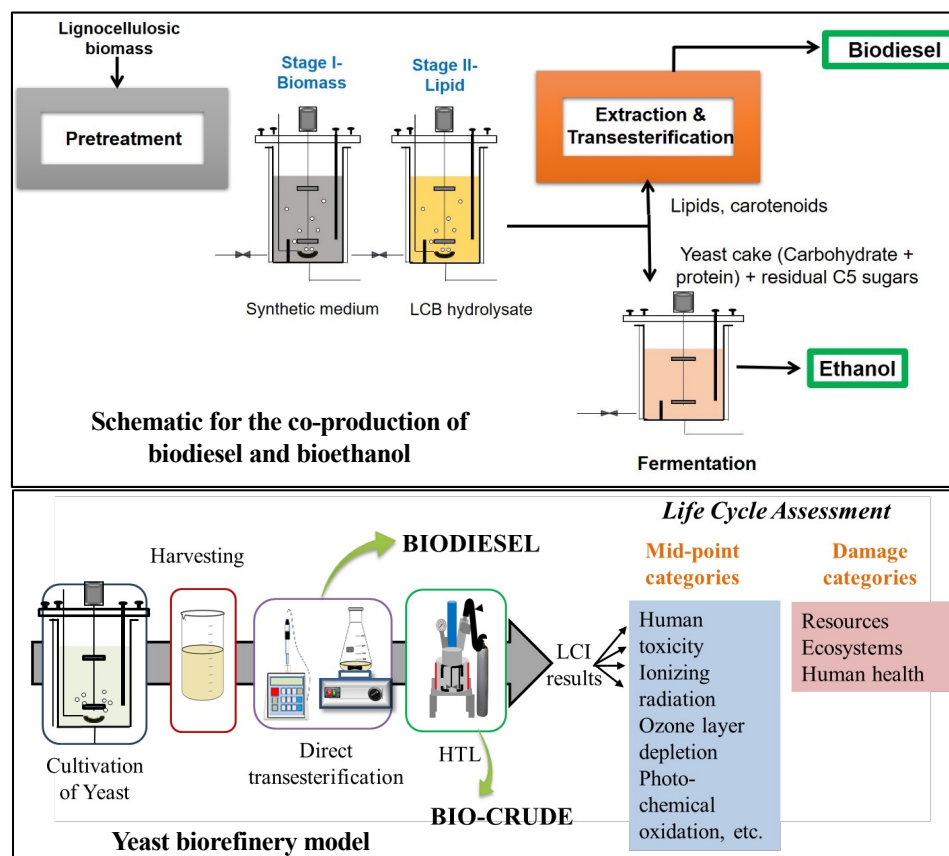
Finite reserve of fossil fuel along with global climate change have urged research and development into the field of renewable fuel production. Although various kind of feedstock have been tried, the sustainability, commercial viability of the process and its capability to meet the global fuel demand is still a question. Agro-industrial waste, rich in functional and valuable compounds, has gained attention as a renewable feedstock for the production of an array of chemicals that can serve as replacements for petro-chemicals. India being an agriculturally rich country, agro-waste holds significant promise for use as a feedstock for production of biofuels. My research focusses on biofuel production (energy dense products like bioethanol, biodiesel or biocrude) by fermentation or hydrothermal liquefaction along with valorization of residual waste to high value products like glycerol, biochar, carotenoids, etc. to offset the high biofuel production cost in a biorefinery model.

Sustainability analysis by life cycle assessment (LCA)

The sustainability and economic viability of the process is analyzed by LCA studies. Biofuel, particularly liquid, is one of the most sought-after renewable energy sources that have the potential to substitute fossil fuel primarily because of its greener composition, cleaner combustion, and a wide array of available feedstocks from which it can be produced. Sustainability assessment studies, encompassing multiple aspects such as, environmental, economic, and societal, are a powerful tool and way forward for the commercialization of biofuels. Therefore, the potential for commercialization of biofuel production technology needs to be assessed by life cycle assessment (LCA) studies. The aim is to critically analyze a set of indicators for the identification of the most sustainable and adaptable biofuel production technology.

3G biodiesel production:

Oleaginous microorganisms like yeast and microalgae can store up to 70% lipids in the form of triglycerides intracellularly, which can be then transesterified to fatty acid methyl esters (biodiesel). We aim to identify new strains with high lipid accumulating properties.



Optimization of pretreatment methods for LCB:

LCB is very recalcitrant in nature and the pretreatment methods employed prior to biofuel production accounts for the primary cost of its production. Hence, novel greener methods should be adopted coupled with LCA and cost analysis to assess its viability in larger scale.

Selected publications:

- J. Chopra, V. Rangarajan and R. Sen. Recent developments in oleaginous yeast feedstock based biorefinery for production and life cycle assessment of biofuels and value added products. *Sustainable Energy Technologies and Assessments*, 53 (2022), pp. 102621
- J. Chopra, B.R. Tiwari, B. K. Dubey and R. Sen. Environmental impact analysis of oleaginous yeast based biodiesel and bio-crude production by life cycle assessment. *Journal of Cleaner Production*, 2020, 271, 122349.
- J. Chopra, D. Mahesh, A. Yerrayya, R. Vinu, R. Kumar and R. Sen. Performance enhancement of hydrothermal liquefaction for strategic and sustainable valorization of de-oiled yeast biomass into green bio-crude. *Journal of Cleaner Production*, 227 (2019), 292-301