భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్ भारतीय प्रौद्योगिकी संस्थान हैदराबाद Indian Institute of Technology Hyderabad

## CHEMICAL ENGINEERING DEPARTMENTAL BROCHURE

INDIAN INSTITUTE OF TECHNOLOGY, HYDERABAD

Department website: https://che.iith.ac.in



🔰 @che\_iith

## TABLE OF CONTENTS

HOD's Message	2
Chemical Engineering @ IITH	3
Academic Programs	4
B.Tech – Course Curriculum	6
M.Tech – Course Curriculum	7
Elective Courses	8
Research Areas	9
Research Themes	10
Faculty Profiles	17
Department Staff	39
Research Facilities	40
University & Industry Collaboration	41
Faculty Achievements	42
Student Achievements	43
Gallery	44



#### HEAD OF DEPARTMENT'S MESSAGE



Welcome to the Department of Chemical Engineering at IIT Hyderabad (ChE@IITH). On behalf of the department, it is my great privilege to present this wonderful stream of engineering to you. ChE@IITH is one of the fastest growing Chemical Engineering Departments in the country and has an excellent reputation in teaching and research, built over the last 14 years.

Our aim is to provide an excellent and accessible chemical engineering education program that is tailored to address technology challenges of the real world. Our dream is to become a department from which future technology leaders of the modern world will emerge. We hope to achieve our objective and fulfill our dreams with the help of young and vibrant team of faculty members, technical staff and scholars. Our core values of responsible training, integrity and mutual respect are the primary pillars on which the department stands. I believe that with these core values we can build centers of excellence from which future technology leaders will emerge.

Faculty from the department actively address challenges in the fields of health, energy security and national security. We address these challenges by utilizing our research expertise in a range of domains like- Advanced Materials, AI/ML, Biofuels, Catalysis, Drug Delivery, Fuel Cells, Mineral Processing, Nanoengineering, Polymer Engineering, Soft Matter and Systems Biology. The web pages of the department provide more information about the programs, facilities and the faculty members. Please reach out to the office of Chemical Engineering(office@che.iith.ac.in) or the faculty members if you have any queries about the programs in the department and the research facilities.

Sincerely,

Balaji Iyer Head of Department, Chemical Engineering head@che.iith.ac.in

#### CHEMICAL ENGINEERING @ IITH

Chemical Engineering at IITH (ChE @ IITH) is one of the fastest growing ChE departments in the country. With 22 faculty members engaged in cutting edge research, we provide quality programs in chemical engineering education, research, and expert consulting support to process industries.

## VISION

"To be recognized by academia and industry as the country's top department for chemical engineering education and research and be the preferred place for students, recruiters and faculty in their quest for learning, identifying the next generation scientists and research freedom."





## MISSION

"To deliver world-leading research, education, and inspiration in chemical engineering and practice what we learn as a chemical engineer to serve the country and society at large, catalyzing transformations in industry and society"

#### ACADEMIC PROGRAMS



#### INTERDISCIPLINARY GRADUATE PROGRAMS

Faculty in ChE @ IITH are also engaged in several interdisciplinary programs. This includes, for example, MTech in Polymer and Biosystems Engineering, Climate Change, Additive Manufacturing, E-Waste Resource and Engineering Management.

### CORE CHEMICAL ENGINEERING ACADEMIC PROGRAMS

ChE @ IITH offers BTech, MTech and PhD programs. The core curriculum builds strong foundations in chemical thermodynamics, reaction kinetics, fluid mechanics, process control, principles of heat and mass transfer, and transport phenomena. The department electives that encompass the state-of-the-art topics in chemical engineering spanning materials, energy, healthcare and computing along with training on live projects prepare our students to address problems that cut across the boundaries of conventional chemical engineering.



#### B.Tech

#### Features:

- Total credit requirement is 129
- B.Tech (Hons) is also offered by the department
- A project work is compulsory for B.Tech (Hons) students
- Students can opt for ChE as minor or major through earning specified additional credits

Duration: 4 years (8 Semesters)

Entrance: Admission through JEE Advanced

#### Dual Degree (B.Tech + M.Tech)

#### Features:

- A student can choose to continue for higher program by converting to dual degree
- Masters thesis is compulsory for all dual degree students
- Dual degree students are eligible to receive fellowship in the last two semesters as per regular M.Tech students

Duration: 5 years (10 Semesters)

Entrance: Admission through JEE Advanced

#### **Regular M.Tech**

#### Features:

•

- Total credit requirement is 52, which includes 17 core courses, 7 electives, and 4 laboratory courses
- M.Tech thesis credit requirement is 24
- Several M.Tech thesis topics are motivated by the industry
- Industry lectures have been introduced in the M.Tech curriculum to get students acquainted with different topics of industry interest

#### Duration: 2 years (4 Semesters)

B.E/B.Tech with valid GATE score

department specified cut off CGPA

M.Sc with UGC/CSIR NET and

Entrance: Admission through GATE, IIT graduate with minimum CGPA 8.0 without GATE score

#### Self-Sponsored M.Tech

#### Features:

- Self sponsored M.Tech is non-subsidized master's degree program.
- Academic requirement is similar to the regular M.Tech program.
- Candidates are required to pay tuition fees on per credit basis.
- Such candidates are not eligible for financial assistantship under MoE.

Duration: 2 years (4 Semesters)

*Entrance:* Minimum CGPA 7.0 and based on the performance in written test and interview

Direct PhD	Regular PhD				
Features: Total credit requirement is 24	Features: Total credit requirement is 12				
Duration: 5 years with Fellowship	Duration: 5 years with Fellowship				
Eligibility criteria:	Eligibility criteria:				

- M.E/M.Tech with department specified cut off CGPA or equivalent
- IITH project sponsored candidates are also eligible to apply

#### External/Sponsored PhD

#### Features:

- Total credit requirement is 24
- Candidates from national laboratories, academia and industry are eligible.

Duration: 5 years with no Fellowship

*Eligibility criteria*: M.E/M.Tech with minimum 2 years of experience

# **M.TECH**

ECH

m

## DHD

## **BASIC SCIENCES**

- Modern Physics
- Environmental Chemistry
- Calculus-I
- Calculus-II
- Applied Chemistry
- Chemistry Lab
- Life Science
- Elementary Linear Algebra
- Differential Equations

## **BASIC ENGINEERING**

- Digital Fabrication
- Thermodynamic Laws & Phase Transitions
- Basic Electrical Engineering
- Materials Science for Chemical Engineers

## MODELLING & SIMULATION

- Numerical Methods
- Applied Mathematics in Chemical Engineering
- Process Control

## SOFT SKILLS

- English Communication
- Introduction to Entrepreneurship
- Personality Development

## DEPARTMENT CORE COURSES

- Introduction to Chemical Engineering
- Chemical Process Calculations
- Biological Engineering
- Transport Phenomena
- Chemical Engineering Thermodynamics
- Chemical Reaction Engineering-I
- Heat transfer
- Fluid Mechanics
- Mass Transfer I
- Mechanical Operations
- Chemical Technology
- Chemical Reaction Engineering-II
- Mass Transfer II
- Process Design and Economics
- Process Intensification

## **COMPUTER SCIENCE**

- Introduction to Programming
- Intro to Al& ML

## **B.TECH**

### **SEMESTER-1**

- Advanced Numerical Methods
- Heterogeneous Catalytic Reaction Engineering
- Advanced Process Control
- Process Integration
- Process Engineering Lab
- English Communication
- Electives

## SEMESTER-2

- Advanced Transport Phenomena
- Molecular Thermodynamics
- CFD Lab
- Industry Lectures
- Thesis (Stage 1)
- Electives

**M.TECH** 

## **SEMESTER-4**

Thesis (Stage 3)

SEMESTER-3

Thesis (Stage 2)

#### **ELECTIVE COURSES**

A unique feature of the department's academic program is its carefully curated list of electives that expand the curriculum beyond the foundations presented via the core courses. The electives expose students to the present multi-disciplinary state of the field of chemical engineering which underpins materials, health care and energy science and engineering. Our electives cover these state-of-the-art fields and help prepare students to be competent to engage in industrial, research or academic careers of their liking.

#### Materials and Health Sciences Research

- Engineering Materials
- Interfacial Chemistry
- Introduction to Nanotechnology
- Intermolecular Forces
- Surface Interactions
- Physico-chemical Fundamentals for Chemical Engineers
- Introduction to Microfluidics and Microreactors
- Food Rheology
- Membrane Separation Process
- Fluidization Technology
- Colloids Emulsions and Foams
- Light Scattering Methods for Complex Fluids
- Fundamentals of Droplet Drying
- Polymer Science and Engineering
- Introduction to Cardiovascular Mechanics

## **ELECTIVES**

#### Computing and Applied Mathematics Research

- Introduction to Statistical Hypothesis Testing
- Machine Learning for Process System Engineering
- Introduction to Stochastic Differential Equations
- Optimization Techniques
- Computational Fluid Dynamics
- Non-Newtonian Fluid Mechanics
- Data Analysis Tools in Experimental Research
- Modern Probability Theory
- Molecular Modelling of Catalytic Reactions
- Linear and Nonlinear Stability of Fluid Flows

#### **Energy Research**

- Chemical Reactor Modelling
- Petroleum Refinery
- Principles of Heterogeneous Catalysis
- Sustainable Energy
- Energy Storage Systems
- Fuel Cell Technology





Faculty	Materials	AI & ML	Bio-engg. & Biotech	Computat ions, DFT, MD		Energy	Fluid Mechanic s	Catalysis	Process Systems	Polymers	Techno- economic s	
Alan Ranjith Jacob	*									*		
Anand Mohan			*				*					
Balaji Iyer			*	*						*		
Chandra Shekhar Sharma	*					*						
Debaprasad Shee								*				
Giridhar Madras	*					*		*				
Kirti Chandra Sahu							*					
Kishalay Mitra		*		*		*			*			
Lopamudra Giri		*	*	*								
Mahesh Ganesan	*									*		
Narasimha Mangadoddy					*		*					
Parag Pawar				*								
Phanindra Jampana		*		*			*		*			
Ramkarn Patne	*						*					
Ranajit Mondal	*									*		
Santhosh Kumar Devarai			*									
Saptarshi Majumdar	*			*						*		
Satyavrata Samavedi	*		*							*		
Shelaka Gupta				*				*				
Suhanya Duraiswamy	*		*			*		*				
Sunil Kumar Maity								*			*	
Vinod Janardhanan						*		*				

Research in the department spans a wide variety of areas including fluids, mineral processing, catalysis, materials for energy and biological applications, nanotechnology, bioengineering, process control, optimization, microfluidics, and DFT studies. Faculties are actively involved in hosting conferences and outreach workshops benefitting the students and faculty across several institutes in India. The Department also houses state of the art research and teaching equipment.

#### CATALYSIS

Our research is focused on the design and development of catalyst materials – ranging from zeolite, and supported metal/metal oxide – with improved reactivity, stability, and selectivity. The catalysts are tested for various industrial processes (e.g., steam reforming, water-gas shift reaction, CO2 conversion and fine chemicals) and biomass-based fuels and chemicals. These studies aim to produce hydrogen, bio-fuels, and value-added chemicals and utilize renewable feed stocks, low-value by-products, and waste materials. The design and optimization of chemical processes using Aspen Plus are an also integral part of this research. An integrated approach considering experimental, and density functional theory (DFT) calculations is applied for rational design of catalyst.



#### ENERGY

The department is at the forefront of pioneering energy research, exploring the realms of biofuels, fuel processing, and novel energy conversion and storage solutions. Our faculty members are fervently engaged in the fundamental and applied dimensions of heterogeneous catalysis; transforming vegetable oils through hydro-deoxygenation, and direct conversion of CO2 into valuable chemicals, steam and oxidative steam reforming of hydrocarbon fuels and biomass conversion to name a few. On the electrochemical side, we are exploring the potential of fuel cells, electrolyzers, and cutting-edge batteries. Our experimental efforts are supported by the power of computational research. This includes the computational identification of novel catalyst materials, intricate reaction pathway analyses, kinetic modeling, and comprehensive reactor modeling for seamless scalability.





#### MACHINE LEARNING IN PROCESS SYSTEMS ENGINEERING

Recent improvements in infrastructures and their affordability, automation, ubiquitous connectivity resulted in generation, processing and management of enormous amounts of heterogeneous data in the domain of Process Systems Engineering (PSE). The research in this direction is to investigate how deep supervised / unsupervised learning methods can be used to solve PSE problems (e.g., surrogate optimization, system identification and control, image-based sensing, uncertainty quantifications, optimal control) more efficiently. Targeted applications are wind farm layout optimization, new alloy discovery, monitoring climate change parameters, fast charging protocols in Li+ battery, bio-fuel supply chain, systems biology to name a few.

#### **RESEARCH THEMES**



#### **FLUID MECHANICS**

We pursue research on a variety of problems of fundamental and applied interest in fluid mechanics, and heat and mass transfer using a combination of tools ranging from basic modeling, computational fluid dynamics (CFD), and linear stability analysis. Fluid mechanics research conducted in the department spans a wide range of topics such as multiphase flows, spatially developing flows in complex geometries, micro-fluidics, and biological flows. A major focus of our research is on understanding the transition to turbulence, with high emphasis on the laminar-turbulent transition.

#### **MINERAL PROCESSING**

In mineral processing research, we are involved in flow sheet development and optimization for various mineral beneficiation plants. We study dense medium cyclones (DMC), hydro-cyclones (HC), feed slurry distributors, grinding mills and flotation devices for understanding the process by using computational modeling techniques (multi-phase CFD/discrete element methods/coupling CFD-DEM models). New innovative/novel improved mineral processing equipment designs through integrated CFD/DEM studies and physical modeling is our major focus. Mathematical models based on industrial data and inputs from CFD/DEM are also being developed using non-linear model building techniques for various mineral processing units.



#### **MOLECULAR & CELLULAR BIOENGINEERING**

The key to understanding the role of chemical engineers in biological engineering research is to recognize that biological systems are inherently chemical in nature. Chemical engineering provides a unique integrated perspective across a wide range of length scales (molecular to macroscopic) that makes it well suited to tackling problems of great interest in modern biology. The thrust of this research theme is to understand and control intercellular interactions and cell-matrix interactions involved in conditions such as inflammation, thrombosis, retinopathy and cancer metastasis. Our efforts are also focused on developing models for vascular processes such as bulk phase intercellular interactions in blood flow.





#### **CARDIOVASCULAR MECHANICS**

Pathologies of the cardiovascular system due to coagulation abnormalities are greatly influenced in their progression by the mechanics of vascular tissue, by the flow behavior of blood in blood vessels, and by the biochemistry of the reactions in the coagulation cascade and fibrinolysis. The thrust of our research is to better understand these pathologies by characterizing the rheological and biochemical variables in flow situations that present in the human vasculature, and by identifying conditions that precipitate potentially life-threating events (like thromboembolisms and strokes). Towards this end, we perform computational simulations of blood flow with suitable complex fluid models of blood in various pathologies. Simulations are validated with experimental data from collaborating groups.

#### **RESEARCH THEMES**



#### **NANOSCIENCE & NANOTECHNOLOGY**

Nanoscience and nanotechnology is a rapidly emerging interdisciplinary field at the interface between physics, chemistry, materials science, electronics, and biology. Broad activities in this fast-changing arena of research include synthesis of a wide range of nanomaterials, their characterization and applications in energy and environment. Presently, we focus on synthesis, fabrication of carbon-based nanostructures and their applications in energy storage devices such as Li ion rechargeable batteries etc. We also deal with nanopatterning of soft matters for various applications such as superhydrophobic surfaces.

#### **DRUG DELIVERY**

Recent advances in materials design offers several new avenues for the development and application of novel materials in drug delivery. This theme is currently focused on developing new methods, materials and technologies to achieve controlled, targeted and sustained release of drugs and cytokines using polymeric biomaterial carriers. We are also interested in investigating mechanisms of drug release and fundamental forces/interactions between polymer and drug molecules. We are equally interested in applying cutting-edge polymer processing techniques that can be used to develop novel drug formulations for application in specialized biomedical domains.



#### **RESEARCH THEMES**

#### POLYMERS

Conventional polymers are currently facing a lot of issues related to the environment as well as their petrochemical origin. Our research program aims to address these aspects by coming up with new grades of environment friendly polymers and/or building knowhow of making biodegradable polymers with customized features for specific applications. The main focus is on building polymerization technoloav through modelina. optimization, and lab scale implementation and then optimally linking with rheology and processing with desired end use properties. Our program also includes research on other polymeric soft materials such as colloids and biopolymers where, we are integrating fundamental, and application driven projects to efficiently create advanced materials of tunable properties.





#### **PROCESS CONTROL & STOCHASTIC CONTROL**

Process Control deals with the use of automatic control strategies to improve efficiency of a chemical process. Apart from the applications of standard control techniques, we develop novel sensor technologies (known as "soft sensors") based solely on data obtained from a running plant. For example, the data could be in the form of images, sound or just input output data of a process stored in a chemical plant. We also study the application of non-linear and stochastic control techniques.



## Alan Ranjit Jacob PhD, University of Crete, 2017

As a member of the 'Soft Matter Group' my focus theme is rheology. We study the physics of flows under deformation and correlate the microstructure and dynamics to bulk flow properties. As a group we are interested in rheology of viscoelastic materials like ketchup, paste, sugar syrup) & viscoplastic materials (like dough). In addition, we have interest in developing rheometric techniques and complex rheological protocols like LAOS to analyse rheological properties of soft materials. We intend to use this expertise in rheology and understand processing techniques like sheeting, spreading & 3D printing

#### πάντα ρεi : everything flows & 'Rheology' is the technique used to study deformation of soft matter

#### Areas of Interest

Food Rheology, Colloids, 3D printing

#### **Research Areas**

- 1. Microgel reversible thermoelectroadsorption: Can colloidal microgels be used as reversible adsorbents to remove 'charged' contaminants from water? We study the physics of colloidal thermoelectroadsorption by PNIPAm microgels on charged contaminants.
- 2. Dough rheology: 2023 is celebrated as the international year of millet, a crop very suitable for semi arid regions like Telangana. Can rheology of the dough provide insights into processing methods like sheeting to facilitate commercial production of millet chapattis?
- 3. Rheology of plant-based butter substitutes: In order to address the sustainability food goals of UN, we are formulating a plant derived butter substitute. Extensive characterizations and rheological studies are done on in house developed formulations to identify a butter substitute that be launched into commercial market.
- 4. 3D printing of highly viscous material: High energetic materials requires to be remotely 3D printed for safe operations. Rheological parameters are linked to processing characteristics like flowability and extrusion-ability, required for developing the ink cartridges and sludge formulations for additive manufacturing.

- 1. Kavya, M., Jacob, A. R., & Nisha, P. (2023). Pectin emulsions and emulgels: Bridging the correlation between rheology and microstructure. Food Hydrocolloids, 143, 108868.
- 2. Jacob, A. R., Parekh, D. P., Dickey, M. D., & Hsiao, L. C. (2019). Interfacial rheology of gallium-based liquid metals. Langmuir, 35(36), 11774-11783.
- 3. Jacob, A. R., Moghimi, E., & Petekidis, G. (2019). Rheological signatures of aging in hard sphere colloidal glasses. Physics of Fluids, 31(8).





## Anand Mohan PhD, Texas A&M University, College Station, 2005

We develop and apply mathematical models and computational tools to study problems in Cardiovascular Mechanics and Complex Fluid Rheology. We use these to propose hypotheses and workflows that can be tested by experiments and clinical practice, respectively.

"Interdisciplinary, problem-focused approaches yield new insights into the behaviour of biological tissues in health and disease."

#### **Areas of Interest**

Cardiovascular Mechanics, Complex Fluids Rheology

#### **Research Areas**

- 1. Efficient software to detect atherosclerosis: Sequential code developed for blood flow is time-consuming and unsuited for use by doctors. We seek to enhance the speed of the sequential code by parallelism and develop a workflow using patient CT scans.
- FEM for blood flow with clot formation in a flexible-walled artery: We seek to demonstrate the potential of any commercial software for clinical use by testing it for a specific fluid-solid interaction problem. The solid zone grows as clotting takes place.
- 3. Hybrid FEM for 2D Blood flow in a flexible tube: The time-consuming nature of numerical fluid-solid interaction studies is sometimes due to the different methods used for fluid vs. solid. An integrated hybrid FEM is sought to be developed and optimized for use with multiple cores.
- 4. A new fluid model that mimics viscoplastic fluids: Conventional viscoplastic "fluid" models have a yield stress term that contradicts the definition of a fluid. They are also difficult to implement in 3D flows. The new fluid model proposed shows promising results in classical BVPs and has been used in a CFD study.

- 1. Anand M, Panteleev MA, & Ataullakhanov FI (2022). Computational models of hemostasis: Degrees of complexity, Applications in Engineering Science, 10: 100103.
- Ameenuddin M, & Anand M (2020). A mixture theory model for blood combined with low-density lipoprotein transport to predict early atherosclerosis regions in idealized and patient-derived abdominal aorta, Journal of Biomechanical Engineering, 142(10): 101008.
- 3. Anand M, Kwack J, & Masud A (2013). A new generalized Oldroyd-B model for blood flow in complex geometries, International Journal of Engineering Science, 72:78-88.







Balaji Iyer VS PhD, IIT Bombay, 2010

Physical and chemical properties of material systems depend on the underlying microstructure and hierarchy of interactions associated with the constituents of the system. Our research is focused on developing tools to study the intricate connection between hierarchical structure, interactions, and the resulting material properties in soft matter systems.

Exploring soft matter using hard science – Building sophisticated tools for probing multicomponent material systems using multiscale simulations.

#### Areas of Interest

Polymers, Nanocomposites, Rheology, Biomimetics





PGN networks

#### **Research Areas**

- 1. Polymer Theory and Simulations: We employ concepts from mechanochemistry, self-consistent field theory and polymer physics to develop mathematical models and multiscale simulations. The models are used for computational design of advanced materials.
- 2. Novel Nanocomposites: We develop advanced computational frameworks to connect microstructure to mechanical properties in synthetic polymer-particle hybrid materials. We are particularly interested in systems with biomimetic structural motifs and complex hierarchical organization.
- 3. Rheology of multicomponent systems: We study structure-rheological property relationships in multicomponent systems with interactions spanning multiple length and time scales. The studies are employed for designing mechanomutable materials.
- 4. Biomimetics: We translate principles of design in biological systems into mathematical models for design of novel materials with desirable properties. We are particularly interested in computational design of self-healing and stimuli-responsive smart materials.

- 1. Iyer, B. V. S., Effect of functional anisotropy on the local dynamics of polymer grafted nanoparticles, Soft Matter, 18, 6209-6221 (2022).
- 2. Kadre D. and Iyer, B. V. S., Modeling Local Shear Dynamics of Functionalised Polymer Grafted Nanoparticles, Macromol. Theory. Simul. 2100005 (2021).
- 3. Iyer, B. V. S., Yashin, V. V. and Balazs, A. C., Harnessing Biomimetic Catch Bonds to Create Mechanically Robust Nanoparticle Networks, Polymer, 69, 310-320 (2015).



## Chandra Shekhar Sharma PhD, IIT Kanpur, 2011

Creative & Advance Research Based On Nanomaterials (CARBON) Lab at IIT Hyderabad is actively engaged with synthesis of a variety of functional nanomaterials (carbon, polymers, metal oxide/sulfides and their composites) including electrospun nanofibers with their application in energy storage (Li-ion, metal-S, metal-CO2 batteries, Supercapacitors), environment, sensors and healthcare.

Creativity, diversity, serendipity and novelty define our approach to solve engineering challenges without fear of failure.

#### Areas of Interest

Nanomaterials, Energy Storage, Sensors, Drug Delivery

#### **Research Areas**

- 1. Metal-CO2 Battery: We use CO2 as an energy carrier to develop indigenous Metal-CO2 batteries for India's Mars mission. In parallel, this research also involves utilizing the excess CO2 from the earth's atmosphere that cause global warming and climate changes.
- 2. Li-ion, Metal-S Batteries & supercapacitors: A number of polymer and biomass precursors are pyrolyzed to prepare carbon electrodes for Li-ion, Metal (Li/Na/K)-sulfur batteries and supercapacitors. Besides materials, we are also working on electrode design (3-D and beyond).
- 3. Gas Sensors: Metal oxide based electrospun nanofibers are being tested for the detection of hazardous gases like H2S at lower temperature. Dopants are used to create hetero p-n junction for enhanced detection even at lower conc.
- 4. Nanofibers based Drug Delivery Systems: We use electrospun nanofibers for controlled drug delivery especially for the oral formulation of hydrophobic and amphiphilic drugs such as Amphotericin-B. Besides, we also work on transdermal patches, wound dressings

- 1. V.K.Bharti, C.S.Sharma, M.Khandelwal, Carbonized Bacterial Cellulose as Free-standing Cathode Host & Protective Interlayer for High performance K-S batteries with enhanced kinetics & stable operation, Carbon, 2023, 212, 118173.
- A.K.Chourasia, A.D.Pathak, C.S.Bongu, K.Manikandan, S.Praneeth, K.M.Naik, C.S.Sharma, In Situ/Operando Characterization Techniques: The Guiding Tool for the Development of Li-CO2 Battery, Small Methods 2022, 2200930
- 3. M.M.Gaikwad, K.K.Sarode, A.D.Pathak, C.S.Sharma, Ultrahigh rate & high-performance Li-S batteries with RF xerogel derived highly porous carbon matrix as cathode host, Chem. Eng. J., 2021, 425, 131521.







## Debaprasad Shee PhD, IIT Kanpur, 2008

Our research group focuses on understanding the catalysis science of mixed metals and metal oxides for various catalytic applications such as production of fuels and chemicals from renewables sources, CO2 conversion, activation of lower hydrocarbons, production and chemical storage of hydrogen. Our research also aims to identify the catalytic active sites existing on the heterogeneous catalyst surface to establish structure-activity/selectivity relationships.

Catalysis has become ubiquitous in our everyday lives and continues to make the world better. Most of the produced commodities involve catalytic transformations.

#### Areas of Interest

Heterogeneous catalysis, Reaction engineering, Mixed metals and metal oxides catalysis, Energy and Environment

#### **Research Areas**

- 1. Catalysis over supported metals and metal oxides: Several supported mixed metals and metal oxides catalysts are developed for various catalytic applications. We aim to identify catalytic active sites to establish structure-activity/ selectivity for rational design of catalysts.
- 2. Energy and Environment: Sustainable production of energy offsets the need of nonrenewable sources and conserve the environment. We aim to develop process and materials for the production of clean energy and their storage. Presently our group is engaged in production of clean hydrogen and transformation of CO2 to fuels and chemical.
- 3. Sustainable production of chemicals: Green carbon feedstocks are required to defossilise the manufacture of bulk chemicals. We aim to develop catalysts and process for the sustainable production of chemicals from renewable sources such as biomass derived feedstocks and other green chemicals.
- Kinetics and reaction engineering: We aim to explore mechanistic aspects of different catalytic and non catalytic chemical reactions, impact of various process parameters, process optimization and operation of reactor.

- 1. Raikwar D., Majumdar S., and Shee D. "Synergistic effect of Ni-Co alloying on hydrodeoxygenation of guaiacol over Ni-Co/Al2O3 catalysts" Molecular Catalysis 499, 111290 (2021).
- Palla V.C.S., Shee D., and Maity S.K "Production of aromatics from n-butanol over HZSM-5, H-Beta, and γ-Al2O3: Role of silica-alumina mole ratio and effect of pressure" ACS Sustainable Chemistry & Engineering 8, 15230-15242 (2020).
- 3. Raikwar D., Majumdar S., and Shee D. "Thermocatalytic depolymerization of Kraft lignin to guaiacols using HZSM-5 in alkaline water-THF co-solvent: A realistic approach" Green Chemistry 21, 3864-3881 (2019).





## Devarai Santhosh Kumar PhD, IIT Madras, 2010

Production of therapeutic enzymes (L-Asparaginase and Lipase), Edible mycelial biomass and Bioactive metabolites from Fungal sps by Sub-Merged (SmF) and Solid-State Fermentation (SSF). Application of metabolites as a promising drug for Malnutrition, Anti-Cancer, and Anti-COVID-19. Fungal Lipase production and its Application for Biodiesel Synthesis. Detection of toxic analytes through hybrid Nanomaterial at ambient temperature.

Edible fungi for Nutritive and Medicinal applications for anti-diabetic, anti-inflammatory and anti-Covid-19. Cost-effective process development for biodiesel

#### Areas of Interest

Bioactive compounds, Therapeutic Enzymes, Bioreactor studies



#### **Research Areas**

- 1. Edible Fungi for Bioactive Compounds: Identification of ergosterol and gallic acid from fungal mycelium as promising anti-COVID-19 metabolites. Purification of Biomolecules, Nutraceuticals and Recombinant Proteins.
- 2. Fungal Enzymes for Therapeutics: Collection, Isolation and Screening of fungal species. L-asparaginase for chemotherapy applications as well as in food processing industries. Scale-up studies and growth kinetics of L-asparaginase in bioreactor.
- 3. Lipase and Biodiesel Synthesis: Prosopis juliflora as a novel substrate to produce lipase by SSF. Developed to separate and quantify the methyl esters (MeP and MeO) in RP-HPLC for accurate analysis. Immobilized lipase used to waste cooking palm oil and found the biodiesel yield.
- 4. Sustainable bio-materials: Mycelium based material for applications in packaging and fabrics. Mycelium binds the agro-waste to obtain a rigid and compact composite material. Bio-Nano sensor, which can detect NO2 at room temperature with extreme precision.

- 1. Hamza, Arman., Ghanekar, Shreya., Kumar, D.S. Current trends in health-promoting potential and biomaterial applications of edible mushrooms for human wellness. Food Bioscience. 51, 102290 (2023)
- Ashok, A., Doriya, K., Rao, J.V., Qureshi, A., Tiwari, A., Kumar, D.S. Microbes Producing L-asparaginase free of glutaminase and urease isolated from extreme locations of Antarctic soil and moss. Scientific Reports. 9, 1423 (2019).
- 3. Gopalakrishnan, L., Doriya, K., & Kumar, D. S. Moringa oleifera: A review on nutritive importance and its medicinal application. Food Science and Human Wellness, 5(2), 49-56 (2016).



## Giridhar Madras PhD, Texas A&M University, 1994

The aim of the research group is to develop new nanomaterials for energy and environmental applications. We also synthesize novel polymeric materials for applications in water purification and drug delivery. We also work in the area of supercritical fluids and its synthesis for biodiesel and bio lubricants.

We are interested in developing novel materials for applications in the energy and environmental sectors.

#### Areas of Interest

Catalysis, Polymers, Supercritical fluids, Energy

#### **Research Areas**

- 1. Heterogeneous catalysis: We develop several new nanomaterials that are used as catalysts for reactions in the energy and environmental sectors. We also propose new reaction pathways and mechanisms providing us with a method to develop new materials with superior properties.
- 2. Polymers: The emphasis has been to synthesize new polymers and also functionalize them with new nanomaterials. We characterize the morphological structure, examine the molecular structure and incorporate model drugs into the matrix to investigate its evolution into media with time.
- 3. Supercritical fluids: The solubilities of various compounds have been modeled using various empirical relations developed by us. These are based on phase equilibria thermodynamics. We have also synthesized bio lubricants and biodiesel in supercritical fluids for the first time.
- 4. Distribution kinetics: We develop continuous distribution kinetic models for granular mixing, precipitation, simultaneous polymerization and degradation, crystal growth, Ostwald ripening, gelation, attrition and the Avrami equation for crystallization.

- 1. MU Rao, K Bhargavi, G Madras, C Subrahmanyam, Basic metal oxide integrated DBD packed bed reactor for the decomposition of CO2, Chemical Engineering Journal 468, 143671 (2023).
- SA Singh, Y Varun, P Goyal, I Sreedhar, G Madras, Feed Effects on Water–Gas Shift Activity of M/Co3O4-ZrO2 (M = Pt, Pd, and Ru) and Potassium Role in Methane Suppression, Catalysts 13 (5), 838 (2023).
- 3. PP Mon, PP Cho, L Chanadana, KV Ashok Kumar, T Shashidhar, C Subrahmanyam, G Madras, Bio-waste assisted phase transformation of Fe3O4/carbon to nZVI/graphene composites and its application in reductive elimination of Cr (VI) removal from aquifer, Separation and Purification Technology 306, 122632 (2023).







## Kirti Chandra Sahu, FASc PhD, JNCASR, Bengaluru, 2007

Our research primarily focuses on studying the dynamics of raindrops and viscosity-stratified flows. We developed a unique experimental facility that mimics the dynamic atmospheric conditions of raindrops descending from cloud to ground. Our other study addresses mixing, a key feature in most modern industrial processes.

Our research provides a much-needed understanding of raindrop shape and size distributions at various altitudes, enabling accurate weather forecasting and climate modelling.

#### Areas of Interest

Raindrops, Bubble dynamics, Stratified flow

#### **Research Areas**

- 1. Raindrops: Accurate rainfall prediction is one of the grand challenges in environmental research due to its relevance in understanding climate change and its accompanying socio-economic impacts, but it is far from perfect. Our research provides important information on the three-dimensional shape, velocity, and size distributions of raindrops for weather forecasting and enables more accurate rainfall prediction.
- Bubble dynamics: Despite being a classic subject that has intrigued scientists for centuries, we were the first to produce a regime map demarcating different bubble rise behaviours, including the previously unknown break-up bubbles.
- 3. Stratified flow: We illustrated how viscosity variation in space and time could profoundly and unexpectedly alter fluid flows. Our study contributed to the comprehension of core-annular pipe flows relevant to the oil and gas industries.

- 1. S. S. Ade, L. D. Chandrala and K. C. Sahu, Size distribution of a drop undergoing breakup at moderate Weber numbers, Journal of Fluid Mechanics, 959, A38 (2023).
- 2. P. K. Kirar, S. K. Soni, P. S. Kolhe and K. C. Sahu, An experimental investigation of droplet morphology in swirl flow, Journal of Fluid Mechanics, 938, A6 (2022).
- 3. K. C. Sahu, A new linearly unstable mode in the core-annular flow of two immiscible fluids, Journal of Fluid Mechanics, 918, A11 (2021).
- 4. R. Govindarajan and K. C. Sahu, Instabilities in viscosity-stratified flow, Annual Review of Fluid Mechanics, 46, 331-353 (2014).





## Kishalay Mitra PhD, IIT Bombay, 2009

The relentless endeavor in Global Optimization and Knowledge Unearthing Lab (GOKUL) is to develop novel methodologies in optimization/machine learning (ML) and apply them while solving various socially relevant and challenging engineering problems. Applications include optimization of wind/bio-energy/H2 energy production under uncertainty, new alloy discovery, monitoring climate change parameters, fast charging protocols in Li+ battery, optimal vaccine production, crop health monitoring etc.

Our research is a humble effort towards exploiting the fascinating journey of Machine Learning for solving socially relevant engineering problems and exploit it to the best of our society's need.

#### Areas of Interest

Process Optimization, Uncertainty, Machine Learning, Supply Chain, Climate Change, Energy, Managing e-Waste

#### **Research Areas**

- 1. Robust design of wind farms: Criticized for inconsistent outputs, wind farms are designed through our novel forecasting, Large Eddy Simulation & ML based wake modeling and data-driven robust optimization techniques, providing realistic bounds on consistent power generation under uncertainty.
- 2. Deep Neural Networks for novel materials discovery: Unveiling process-structure-property relationship is deeply involved when explored by experimentation/high fidelity simulation. Deep learning based our inverse optimization approach can be winner.
- 3. India-wide bio supply chain design: Tapping huge biomass generated in India, this waste-to-wealth generation research talks about how to optimize the entire supply chain through techno-economic-environmental & uncertain factor considerations helping the country's move towards energy self-reliance.
- 4. ML driven optimal vaccine production: Challenging batch operation, better control profiles for vaccine production can be achieved through our bioreactor semi-batch optimization offering by Bayesian inference.

- 1. Gumte, K., Pantula, P. D., Soumitri M. S., Mitra, K., Achieving Wealth from Bio-Waste in a Nationwide Supply Chain Setup under Uncertain Environment through Data Driven Robust Optimization Approach, Journal of Cleaner Production 291, 125702 (2021).
- 2. Mittal, P., Mitra, K., Kulkarni, K., Optimizing the number and locations of turbines in a wind farm addressing energy noise trade-off: A hybrid Approach, Energy Conversion and Management, 132C, 147-160 (2017).
- 3. Ravi Kiran, I., Soumitri M. S., Mitra, K., Deep Learning Based Dynamic Behaviour Modelling and Prediction of Particulate Matter in Air, Chemical Engineering Journal, 426, 131221 (2021).





## Lopamudra Giri PhD, University of Iowa, 2009

The broad research theme of the group is around developing live imaging techniques to study dynamic response in cell systems. Cell-based disease models are devised for testing drugs for neurodegenerative diseases. Further we aim to build a digital twin of the experimental system by integrating Machine learning and Systems biology approach.

Integration of Time-lapse Microscopy and Systems Biology in understanding neurodegenerative diseases

#### **Areas of Interest**

Live cell imaging, Systems Biology, Image analysis

#### **Research Areas**

- Cellular Engineering: Application of engineering approaches to develop quantitative understanding of cell function and apply this understanding for deciphering the action of drugs. This approach was used to identify calcium channel blockers as potential anti-stroke drug.
- 2. Live cell imaging and quantitative microscopy: Development of live imaging techniques using confocal microscopy to measure dynamics of protein aggregation. This approach leads to observe the intracellular phase separation under neurodegenerative condition.
- 3. Disease models: Construction of cell-based disease model based on hypoxia/hyperglycemia and drug testing. Implementation of deep learning models for automated image segmentation.
- Systems Biology: Construction of mathematical model for signaling network and parameter estimation using Monte Carlo sampling. Development of digital model of cell systems using machine learning and biophysical models.

- V. Dhyani, S. Kumar, S.R. Manne, I. Kaur, S. Jana, S. Russell, R. Sarkar, L. Giri, "Three-Dimensional Tracking of Intracellular Calcium and Redox State during Real-Time Control in a Hypoxic Gradient in Microglia Culture: Comparison of the Channel Blocker and Reoxygenation under Ischemic Shock", ACS Chemical Neuroscience, vol. 14(10), pp. 1810–1825. 2023.
- 2. Aishee Dey, Suman Gare, Sarpras Swain, Proma Bhattacharya, Vaibhav Dhyani, Lopamudra Giri and Sudarsan Neogi. "3D imaging and quantification of PLL coated fluorescent ZnO NP distribution and ROS accumulation using laser scanning confocal microscopy." AIChE Journal, vol. 68(9), pp. e17801, 2022.
- Suman Gare, Soumita Chel, TK Abhinav, Vaibhav Dhyani, Soumya Jana and Lopamudra Giri. "Mapping of structural arrangement of cells and collective calcium transients: an integrated framework combining live cell imaging using confocal microscopy and UMAP-assisted HDBSCAN-based approach". Integrative Biology, vol. 14, pp. 184-203, 2022.





## Mahesh Ganesan PhD, University of Michigan, Ann Arbor, 2015

We are part of the Soft Matter Group @ ChE IITH. Understanding the correlation between the microscale structural properties and the macro-scale rheological and optical properties of soft materials (e.g., colloidal gels, polymer solutions, adhesives, biopolymers etc.) is the broad theme of our research group. We seek to apply these understanding to develop 'inverse' design paradigms for realizing soft materials with tailored functional properties.

Soft matter – ubiquitous in natural and industrial systems – are interesting materials that constantly challenge our fundamental understanding.

#### **Areas of Interest**

Soft Matter, Complex Fluids, Modeling, Novel Materials





100





#### **Research Areas**

- 1. Colloidal gels of tunable elasticity: Aggregating particles form a remarkable fractal like network that exhibits a solid like rheology. We seek to discover modes for tuning the linear and non-linear elastic rheology of these materials
- 2. Annealing anisotropic colloidal assemblies: Colloidal particle assemblies are sought for their brilliant structural coloration. Anisotropy in particle shape gives rise to richer color response. Yet, anisometric assemblies are prone to defects. We seek to develop techniques to anneal such crystal defects.
- 3. In situ physics of biofilm polymers: Biofilms are bio-soft materials made of bacterial cells embedded in an extracellular polymeric substance (EPS). I seek to fundamentally understand how the EPS polymers are surprisingly tailor made to suit the biofilm's growth environment.
- 4. Rheological paradigm for vibration damping adhesives: Sticky polymers can interestingly damp vibrational amplitudes in substrates. We aim to develop rheological guidelines for producing polymers that can achieve target damping performances.

- 1. Beckwith, J.K., Ganesan, M., VanEpps, J.S., Kumar, A. and Solomon, M.J. "Rheology of Candida albicans fungal biofilms" Journal of Rheology 66, 683 697 (2022)
- 2. Kao, P.-K., Solomon, M.J.\* and Ganesan, M.\* "Microstructure and elasticity of dilute gels of colloidal discoids" Soft Matter 18, 1350 – 1363 (2022)
- 3. Milliman, Henry W; Ganesan, Mahesh. Multilayer constrained-layer damping, US Patent No. US 11,059,264 B2, July 13, 2021



## Narasimha Mangadoddy PhD, JKMRC University of Queensland, 2010

The broad application of computational techniques such as CFD and DEM to particulate flows in chemical, mineral processing, and energy industries has a huge potential to understand the fundamental flow behavior, particle/disperse phase dynamics and influence of turbulence on separations. We also focus on experimental investigation of the phasic information utilizing process tomography (ERT, PEPT) and imaging techniques.

Understanding the interaction of different phases during the transport processes and separations is an important aspect, provides the scope for thorough insights and new efficient separation devices

#### **Areas of Interest**

Particulate Technology, Mineral Processing, Industrial CFD/DEM, Experimental Fluid Mechanics

#### **Research Areas**

- Development and application of the multi-phase computational models for mineral processing and particulate flows is challenging due to complex interaction of phases apart from their anisotropic turbulence. We develop these via CFD, DEM and coupled approaches.
- Characterizing particulate flows is quite difficult due to its opaque and involved phasic interaction. We seek to measure these via process tomography such as Electrical Resistance Tomography (ERT) and Positron Emission Particle Tracking (PEPT) and imaging.
- 3. Most of the mineral separation units are designed vis trail and error or correlations based. We seek to develop new improved designs using multi-phase CFD and systematic experimental methods. Industrial Cyclones & spirals for coal separation, classification and gravity separation are made via this route
- 4. Currently single avg. density mathematical modes (gravity spns). Multi-component performance models are necessary for performance prediction. We seek to simulate and understand the interactions between the different components using experimental and multiphase CFD methods, which may lead us to develop an improved mathematical models

- 1. T.R. Vakamalla, V.B.R. Koruprolu, R. Arugonda, N. Mangadoddy, Development of Novel Hydrocyclone Designs for Improved Fines Classification Using Multiphase CFD Model, Separation and Purification Technology, 175, 24, 481–497 (2017).
- 2. Balraju Vadlakonda Narasimha Mangadoddy, Hydrodynamic study of three-phase flow in column flotation using Electrical Resistance Tomography coupled with pressure transducers, Separation and Purification Technology, 203, 274-288 (2018)
- 3. Mandakini Padhi, Mayank Kumar, Narasimha Mangadoddy, Understanding the Bicomponent Particle Separation Mechanism in a Hydrocyclone Using a Computational Fluid Dynamics Model, I&ECR, 59, 11621–11644 (2020)





## Parag D Pawar PhD, Johns Hopkins University, 2008

We develop computational frameworks to investigate biophysical responses of multispecies bacterial biofilms to environmental stresses, particularly antimicrobial agents and nutrient starvation.

As bacteria band together to form biofilm communities, the threat of antibiotic resistance poses a formidable threat to the efficacy of our medical interventions.

#### Areas of Interest

Multispecies biofilms, Quorum sensing, Cellular automata





#### **Research Areas**

- 1. Biofilms offer protection against environmental stresses and immune responses. Their high antibiotic resistance poses treatment challenges. Our research aims to uncover the biophysical mechanisms behind this resistance.
- Heterogeneous architecture: The inherent heterogeneity of biofilms, characterized by the presence of distinct microcolonies, plays a pivotal role in eliciting diverse responses to treatment modalities. Our research aims to investigate antibiotic resistance and the emergence of safeguarded microcolonies within developing biofilms.
- 3. Polymicrobial biofilms: A vast majority of infections involve polymicrobial biofilms. We focus on delineating synergistic and antagonistic interspecies-interactions within these biofilms in the context of nutrient competition, quorum-sensing, and phenotypic switching.

- 1. Chirathanamettu, T.R., and Pawar P.D. "Quorum sensing-induced phenotypic switching as a regulatory nutritional stress response in a competitive two-species biofilm: An individual-based cellular automata model." Journal of biosciences 45 (2020): 1-16.
- 2. Machineni, L., and Pawar P.D. "Role of Biofilms in Bioprocesses: A Framework for Multidimensional IBM Modelling of Heterogeneous Biofilms." Horizons in Bioprocess Engineering (2019): 93-112.
- 3. Machineni, L., et al. "A 3D individual-based model to investigate spatially heterogeneous response of biofilms to antimicrobial agents." Math. Methods in the Appl. Sci. 41.18 (2018): 8571-8588.



## Phanindra Jampana PhD, University of Alberta, 2010

The overarching theme of our group is the analysis of stochastic dynamical systems which are ubiquitous in process systems engineering. In this broad area, we study system identification, nonlinear estimation, control, density functional theory and inverse problems. The focus is on developing novel algorithms using tools derived from advanced mathematics and providing guarantees where applicable.

#### Developing mathematical algorithms with guarantees for process systems.

#### Areas of Interest

Inverse problems, System Identification, Control, Estimation



#### **Research Areas**

- 1. Inverse Algorithms in ERT: The main drawback of (electrical resistance tomography is the very low spatial resolution. Our group develops/implements novel reconstruction algorithms deriving from sparse optimization and methods incorporating prior information.
- 2. System Identification: In traditional system identification, the order and the parameters of the model are not found together. In our group, we devise new algorithms that can estimate the parameters and order jointly. Our group incorporates studies the problem tools such as Laplace transform and sparse optimization.
- 3. Nonlinear estimation: Most control designs are based on information of states. However, states are not measure in many applications. Our group uses the particle filters for nonlinear state estimation and study their convergence properties.
- Control of Fluid Systems: Control of fluid systems involves the challenge of partial differential equation models. In our group, we simulate multiphase flow processes using computational fluid dynamics to compute dynamic models for control design.

- 1. Diddi, Suharika; Jampana, Phanindra Varma; Mangadoddy, Narasimha, "Evaluation of Two Non-iterative ERT Reconstruction Algorithms for Air-Core Measurements in Hydrocyclone", Ind. Eng. Chem. Res. 2022, 61, 49, 18017–18029
- Santhosh K. Varanasi and P. Jampana, "Nuclear Norm Subspace Identification of Continuous Time State-Space Models with Missing Outputs", Volume 95, 2020, 104239
- 3. Santhosh K. Varanasi, Manchikatla Chaitanya and P. Jampana "Input Design for Continuous Time Output Error Models", Ind. Eng. Chem. Res. 2019, 58, 26, 11175–11186



## Ramkarn Patne PhD, IIT Kanpur, 2019

Understanding the dynamics of fluid flows is essential in myriad natural and industrial settings ranging from biofluid mechanics to additive manufacturing. The overarching theme of my research group is to analyse the dynamics of flows and apply it to manipulate the hydrodynamic instabilities to achieve the industrial application goal or understand the natural phenomena.

The growth of the perturbations in space and time leads to hydrodynamic instabilities which could lead to the ubiquitous turbulent flow. Thus, control of instabilities is essential in controlling turbulence.

#### Areas of Interest

Hydrodynamic stability, Biofluid mechanics, Complex flows

#### **Research Areas**

- 1. Pulmonary fluid dynamics: We analyse the instabilities involved in the mucus flow vital in leading to the airway closure scenarios. The strategies to mitigate these instabilities is also being explored.
- 2. Buoyancy instabilities: A liquid layer heated from below is known to become unstable as heating temperature is increased beyond a certain value due to buoyancy instability. We analyse the modification of this instability by subjecting the liquid layer to an oblique temperature gradient.
- 3. Flow past deformable surfaces: These flows are encountered in biological and microfluidic settings. We analyse the impact of the deformable surface on flow dynamics and use it to manipulate the mixing.
- 4. Complex flows: Biological and industrial fluids often have a complex relationships between the applied stress and resulting velocity field gradient defined by a constitutive relation. We analyse the impact of non-Newtonian character on hydrodynamic instabilities.

- 1. R Patne, Effect of inhaled air temperature on the mucus dynamics, Journal of Fluid Mechanics, under review.
- 2. R Patne and J Chandrana, Spatio-temporal dynamics of a two-layer pressure-driven flow subjected to a wallnormal temperature gradient, Journal of Fluid Mechanics, 957, All (2023).
- 3. R Patne, Purely elastic instabilities in the airways and oral area, Journal of Fluid Mechanics, 928, A22 (2021).





## Ranajit Mondal PhD, IIT Madras, 2020

As part of the Soft Matter Group @ChE IITH, our broad research theme is the fundamental aspects of colloids & interfacial Science. Our research interests are understanding the evaporative patterning of colloids, fracture mechanism in the colloidal film, Pickering emulsion, and foams, and designing particle-polymer hybrid material. We aim to design sustainable and functional soft materials for food, pharmaceutical, sensing, and separation applications.

Colloids are a broad category of complex materials where interactions between phases and interfaces dominate the system's behavior.

#### Areas of Interest

Colloids, Drying drops, Desiccation cracks, Functional Soft Materials



#### **Research Areas**

- 1. Droplet Drying and Assembly of Colloids: Drying particle-laden drop is ubiquitous. We seek to understand the drying kinetics of a particle-laden drop and investigate the various physical factors that affect the assembly of particles.
- Desiccation cracks in a dried film: Desiccation cracks are quite prevalent in nature, and examples include dried mud, old paintings, colloidal crystals, etc. Using colloids as a model system, we look at the origin of diverse crack morphologies and investigate the possibilities of manipulating the desiccation cracks by employing external fields.
- 3. Capillary suspension, Pickering emulsions, and foams: Designing capillary suspensions, Pickering emulsions, and foams are of interest. We aim to better understand the significance of particle shape and bridge the gap between microstructural change and properties.
- 4. Porous Hybrid Materials: The rapid technological growth paved the way for developing novel materials. Porous hybrid materials are appealing, and we aim to use the ice-templating method to design macroporous hybrid materials and seek to understand their structure-property relations.

- 1. Mondal, R., Lama, H., and Sahu, K.C. "Physics of drying complex fluid drop: Flow field, pattern formation, and desiccation cracks" Physics of Fluids 35, 061301 (2023)
- Das, A., Mondal, R., Sen, D., Bahadur, J., Satapathy, D.K., and Basavaraj, M.G. "Jamming of Nano-Ellipsoids in a Microsphere: A Quantitative Analysis of Packing Fraction by Small-Angle Scattering" Langmuir 38, 12, 3832– 3843 (2022)
- 3. Mondal, R., and Basavaraj, M.G. "Patterning of colloids into spiral via confined drying" Soft Matter 16, 3753-3761 (2020)



## Saptarshi Majumdar PhD, IIT Kharagpur, 2008

Our focus on Poly-Nano-Bio group, is developing cross-linker free biomaterials and understanding the physicochemical aspects of ionic interactions with charged polymers. The chemically modified polymer biomaterials may result in toxicity and issues with biocompatibility and FDA approvals. Hence, we focus on the physical interactions of polymers to develop biomaterials for different applications. We also emphasis on developing certain theories on charged polymers. Our group actively worked with Tata Steel to develop laboratory demonstrations for several products from lowcost tailing coals.

Biomaterials & charged Polymers - A complicated domain with interesting dynamics and applications

#### Areas of Interest

Polymers, Ion interactions, Biomaterials, Molecular dynamics, Industrial Processes

#### **Research Areas**

- Physicochemical aspects of polyelectrolytes and polyampholytes. Biomaterials are prepared using chemically 1. crosslinked polymers to increase their dissolution resistance which in turn induce toxicity. Main emphasis is given to the interactions of the charged polymers to get the desired cross-linker free biomaterials without hampering the biocompatibility.
- 2. Interaction perspective of biomaterial development: The biomaterials are usually developed using the trialand error method and without a scientific knowledge of interactions. The main aim is to study the interactions of polymers and other components and design a better biomaterial showing superior results.
- 3. Ionic interactions of polymers: The theories of polymer physics are more aligned towards the neutral polymers. We aim to develop certain theories by studying the ionic interaction (salts, acids) with charged polymers and an applications of these in biomaterial development.
- 4. Tailing Coal to Value Added Products: Several projects are successfully completed with Tata Steel in last few years to convert waste to wealth i.e., low-cost tailing coal to value added products like C-slurry (as fuel), Activated-C and Battery Grade electrode materials.

#### Selected Publications

- 1. T. Basu, U. Bhutani, S. Majumdar, Cross-linker-free sodium alginate and gelatin hydrogels: a multiscale biomaterial design framework. J. Mater. Chem. B 10, 3614–3623 (2022).
- 2. S. Das, L. Giri, S. Majumdar, Hofmeister series: An insight into its application on gelatin and alginate-based dual-drug biomaterial design. Eur. Polym. J. 189, 111961 (2023).
- 3. T. Basu, S. V Chituru, S. Majumdar, Unraveling fluctuation in gelatin and monovalent salt systems: coulombic starvation. Soft Matter 19, 2486-2490 (2023).
- 4. S K Sriramoju, PS Dash, S Majumdar, Meso-porous activated carbon from lignite waste and its application in methylene Blue adsorption and coke plant effluent treatment. J of Environ. Chemical Engg. 9 (1), 104784, 2021





Salt Concentration



## Satyavrata Samavedi

PhD, Virginia Tech, Blacksburg, 2013

The Electrospun Cellular Microenvironments (ECM) Laboratory is interested in investigating structure-property-processing relationships in polymeric biomaterials for biomedical applications. We study and control the process of electrospinning to rationally design functional polymeric matrices for promoting controlled drug release, creating stable amorphous drug formulations and achieving drug/cytokine combination therapy for immunomodulation.

The design, processing and functionalization of degradable biomaterial matrices: from polymer physics to biomedical applications.

#### Areas of Interest

Polymeric biomaterials, Electrospinning, Controlled drug/protein delivery, Amorphous drug formulations, Immunomodulation

#### **Research Areas**

- 1. Physics of polymer electrospinning: We investigate electrospinning via direct in situ visualization of the cone/jet to gain insights into parameters that influence cone dynamics, jet initiation/stretching and fiber formation. These insights are used to develop fibrous meshes with predictable diameter and specific mesh properties.
- 2. Design of controlled release carriers: We adopt a fundamental approach to understanding the roles of matrix properties that govern the release of small molecule hydrophobic drugs. We build upon this knowledge to design carriers that exhibit controlled and sustained release of immunomodulatory drugs, particularly zero-order kinetics. A growing interest in our group is the development of stable co-amorphous drug formulations.
- 3. Combination therapy for immunomodulation: We develop technologies to process polymers that can simultaneously deliver drugs and proteins while retaining independent control over release of the individual therapeutics and preserving biological functionality. In close collaboration with biologists, we currently target dysfunctional immune responses associated with degenerative diseases.

#### **Selected Publications**

- 1. N Joy, "Coupling between voltage and tip-to-collector distance in polymer electrospinning: insights from analysis of regimes, transitions & cone/jet features", Chemical Engineering Science, 230, 116200, 2021
- 2. D Venugopal et al., "Electrospun meshes intrinsically promote M2 polarization of microglia under hypoxia and offer protection from hypoxia-driven cell death", Biomedical Materials, 16, 045049, 2021
- 3. N Joy et al., "Robust strategies to reduce burst and achieve tunable control over extended drug release from uniaxially electrospun composites", European Polymer Journal, 168, 111102, 2022



IL-4/IL-6 IL-10/IL-6



## Shelaka Gupta PhD, IIT Delhi, 2019

The multiscale modelling in energy and catalysis (MMEC) group at IITH uses quantum mechanical ab initio density functional theory (DFT) simulations for the rational design of heterogenous catalysts used for the sustainable production of fuels, materials and chemicals. The ab initio calculations provides a mechanistic insight of the reaction which helps in engineering the catalyst.

Understanding and designing the atomic scale catalyst features which govern molecular transformations for a wide range of applications.

#### Areas of Interest

Bio renewables, Heterogeneous Catalyst, Molecular Modelling High Entropy Alloys

#### **Research Areas**

- 1. Biomass to value added fuels an chemicals: Developing an integrated fermentation and catalysis process wherein biomass derived platform molecules obtained from the fermentation of waste biomass could be catalytically upgraded to value added fuels and chemicals.
- 2. High entropy alloys: Understanding the diffusion, segregation and oxidation behaviour of high entropy alloys using Density Functional Theory (DFT) and Molecular Dynamic (MD) Simulations
- 3. Reduction of Nitroarenes: Hydrogenation of nitroarenes to aniline is an important route for the synthesis of value-added chemicals, pharmaceuticals etc. DFT simulations in combination with experiments have been used to understand the role of oxygen vacancies on CuO surface in the reduction of nitroarenes to aminoarenes.
- 4. Hydrodechlorination of Chlororganics: Catalytic hydrodechlorination (HDC) has been used as a method for the elimination of chlororganics from wastewater. DFT simulations in combination with Micro kinetic modelling are used for the rational design of transition state metal-based catalyst for the HDC reactions.

- K. Rajendran, J. Yadav, T.S. Khan, M.A. Haider, S. Gupta\* & D. Jagadeesan\* "Oxygen Vacancy-Mediated Reactivity: The Curious Case of Reduction of Nitroquinoline to Aminoquinoline by CuO" J. Phys. Chem. C, 2023, 127, 18, 8576-8584.
- C.S. Shenoy, T.S. Khan, K. Verma, M. Tsige, K.C. Jha, M.A. Haider\* & S. Gupta\* "Understanding the origin of structure sensitivity in hydrodechlorination of trichloroethylene on a palladium catalyst" React. Chem. & Eng., 2021, 6, 2270-2279.
- 3. K. Rajendran, N. Pandurangan, C.P. Vinod, T.S. Khan, S. Gupta\*, M.A. Haider, & D. Jagadeesan\* "CuO as a reactive and reusable reagent for the hydrogenation of nitroarenes", Applied Catalysis B: Environmental, 2021, 297, 120417.





## Suhanya Duraiswamy PhD, NUS Singapore, 2012

Controlled Microenvironments lead to fascinating phenomena that are not obvious in the macroworld we live in. Microfluidics provides us a window to this microworld, and analysis of such properties enable us to develop powerful tools that can, in the long run, be applied to Healthcare and Energy sectors.

Few 100 µm fluidic channels – microfluidics Micro and millifluidic channels are typical PFRs Multiphase flows with bubbles, drops, foams introduce flowing microreaction vessels

#### Areas of Interest

Microfluidics, Theranostics, Sensors, Microphotoreactors, Nanomaterial synthesis and assembly

#### **Research Areas**

- 1. Particle synthesis and assembly: Multiphase micro flows enable automated, reproducible and robust synthesis and/or assembly of the particles due to the control of reagent contacting and their kinetics. Our focus is on plasmonic nanomaterials.
- Pathogen isolation and recognition: Pathogen isolation from body fluids for disease diagnostics and personalized therapy using multiphase flows and pathogen specific protein bound nano-materials within few minutes of sample collection is the objective. The isolated pathogen-protein complex will be then processed using on-chip PCR/LAMP/AI-ML tools
- 3. 3D organoids for personalized therapy: 3D in vitro tumor models such as spheroids and organoids with and without supports are being explored in this research focus. These will be directly extended to high-throughput combinatorial drug testing, delivery and therapy.
- 4. Microphotoreactors: We are currently working towards a platform technology which will later find applications in water treatment, waste to value added products, artificial photosynthesis and other solar-driven applications.

- 1. Suhanya Duraiswamy, Saif A. Khan, "Plasmonic Nanoshell Synthesis in Microfluidic Composite Foams", Nano Letters, 10, 3757–3763 (2010)
- 2. Duraiswamy S., Khan S. A., "Droplet-Based Microfluidic Synthesis of Anisotropic Metal Nanocrystals", Small, 5(24), 2828–2834 (2009).
- 3. Sushama Agarwalla, Suhanya Duraiswamy, "Micro-piezo Actuator for Cell Lysis", Microactuators, Microsensors and Micromechanisms, (2022).





## Sunil K Maity PhD, IIT Kharagpur, 2007

Our research is focused on producing biofuels and bio-based chemicals using the chemo-catalytic approach. The major thrusts are understanding the reaction mechanism and structure-catalytic activity correlation. We also carry out techno-economic and profitability analyses to evaluate their commercial potential.

Hydrocarbon biofuels and building-block chemicals are essential for sustainability.

#### Areas of Interest

Catalysis, Biofuels, Renewable chemical, Techno-economic analysis

#### **Research Areas**

- 1. Hydrocarbon biofuels: Hydrodeoxygenation of vegetable oil, fatty acid, biofuel precursors, etc., in the presence of hydrogen and supported metal catalysts produces hydrocarbon biofuels, which are compatible with current combustion engines.
- 2. Synthesis gas: Reducible oxides, such as CeO2–ZrO2, are important catalyst carriers to improve catalyst stability during the steam reforming reaction.
- 3. Pinch technology: Energy is one of the main operating costs in a chemical process. Process integration using pinch technology is vital to improve the thermal efficiency of a process.
- 4. Techno-economic analysis: Techno-economic and profitability analysis is vital to evaluate the critical economic barriers in the way of commercialization.

#### **Selected Publications**

- 1. SK Maity, K Gayen, TK Bhowmick, Hydrocarbon biorefinery: Sustainable processing of biomass for hydrocarbon biofuels. Academic Press, Elsevier 2021.
- A Kunamalla, SK Maity, Production of green jet fuel from furanics via hydroxyalkylation-alkylation over mesoporous MoO3-ZrO2 and hydrodeoxygenation over Co/γ-Al2O3: Role of calcination temperature and MoO3 content in MoO3-ZrO2. Fuel 2023, 332, 125977.
- 3. Mailaram S., Maity S.K. Dual liquid–liquid extraction versus distillation for the production of bio-butanol from corn, sugarcane, and lignocellulose biomass: A techno-economic analysis using pinch technology. Fuel 2022, 312, 122932.

## HYDROCARBON BIOREFINERY

Sustainable Processing of Biomass for Hydrocarbon Biofuels







## Vinod Janardhanan PhD, University of Karlsruhe, 2007

My research interests are primarily focused on electrochemical devices and heterogeneous catalysis. Specifically, our research is focused on the development and characterization of unitized regenerative fuel cells for energy conversion and storage. When it comes to heterogeneous catalysis, our research aims to develop micro-kinetic and mechanistic models for various reaction systems.

URFC: Unitized regenerative fuel cells can be a paradigm shift in energy conversion and storage because of their scalability and high round trip efficiency.

#### Areas of Interest

Catalysis, Fuel cells, Electrolyzers, Multiscale modeling



0.16

#### **Research Areas**

- 1. HT-PEMFC: We prepare MEA's for HT-PEMFCs. The main focus of the research is the the reduction of Pt loading in the catalyst layer by optimizing the catalyst ink composition and by trying different support materials.
- 2. HT-PEMWE: The main challenge in the anode catalyst, which undergoes corrosion at the cell potentials. We work towards circumventing this problem by using Pt-X/MWCNT and Pt/Conducting polymers.
- 3. Kinetic models: Reliable kinetic models are vital for reactor design and scale-up. We work on the development of kinetic models for various applications. The models include micro-kinetic model as well as mechanistic kinetic models.
- 4. Julia package: A free-to-use Julia package for reacting flow simulations. Rich library: thermochemistry, gasphase and surface kinetics, transport properties. Applications: Batch, Plug, CSTR, Surface coverage, Multicomponent equilibrium etc.

- 1. Prakash V. Ponugoti, Priya Pathmanathan, Jyotsna Rapolu, A. Gomathi, Vinod M. Janardhanan, On the stability of Ni/γ-Al2O3 catalyst and the effect of H2O and O2 during biogas reforming, Appl. Catal. A 651, 119033 (2023)
- 2. Prakash V. Ponugoti, Pritesh Garg, Sanjana N. Geddam, Samik Nag, Vinod M. Janardhanan\*, Kinetics of iron oxide reduction using CO: Experiments and modeling, Chem. Eng. J 434, 134384 (2022)
- 3. Anusree Unnikrishnan, N Rajalakshmi, Vinod M. Janardhanan\*, Kinetics of electrochemical charge transfer in HT-PEM fuel cells, Electrochim. Acta , 293, 128-140 (2019)



#### DEPARTMENT STAFF



Suman Gupta Technical Officer Grade-1



Somesh Rao Nama Technical Superintendent



P Gayathri Technical Superintendent



Veerabhadra Rao Koruprolu Technical Superintendent



Ramireddi Hari Krishna Technical Superintendent



Mr Harish Ramineni Executive Assistant



Nagarjuna Ponnoli Technicia n



Cheemakurthi M Subhani Multi Skill Assistant GR-1



Lalitha Technician



Venkata Krishnaiah Junior Technician



Bharath G Relekar Junior Technician



Kavvampalli Srinivas Junior Technician



#### **RESEARCH FACILITIES**

ChE @ IITH in collaboration with the Japan International Cooperation Agency (JICA) and IITH along with support from faculty project grants has setup several key high-end research facilities that cater to the different research projects in the department. Some of our capital equipment are indicated below. The department faculty maintain these equipment and make them available to faculty across departments for use.

## LIST OF EQUIPMENT

- Scanning Electrochemical Microscope
- Gel Permeation and Size Exclusion Chromatograph Systems
- Biosensor for gas & Humidity testing Unit
- Integrated reverse High performance Liquid Chromatography
- Chemical Reactor below 1 L 500ML, above 1L 2000ML with accessories, spectrophotometer, analytical balance & 3L laboratory fermenter
- Multiple Array Systems for High Throughput Assays
- Circular Dichroism Spectrometer/Polarimeter
- Differential Scanning Calorimetry
- Isamill/Agitator Mill for Fine Grinding
- Force-Sensing Optical Tweezer
- Module Scale Battery Testing System
- Driving Simulator
- Multimode Microplate Reader With Live Cell Imaging Facility
- UPLC-HRMS Systems
- Volumetric PIV Systems & Accessories
- Wire Mesh Sensors System
- Multifunctional High Resolution X Ray Diffractometer (HR-XRD)
- Stereolithography (SLA) Based 3D Production Printer Model Project 6000
- MP-AES Microwave Plasma Atomic Emissions Spectrometer
- HPC Cluster-250 Crores
- Rheometer with different geometry and accessories
- Confocal Laser Scanning Microscope with Incubation Chamber
- Dynamic light scattering and zeta potentiometer







Faculty in the department are engaged in several collaborative research projects with industry, other academic institutions both within and outside the country as well as contributing to several national missions via joint projects with governmental research establishments such as DRDO.

**FUNDING AGENCIES SUPPORTING RESEARCH IN CHE @ IITH** 



... and many more

For more details, please check our departmental website

#### **Research – Journal Editorship**

- Dr. Chandra Shekhar Sharma has been inducted in the Editorial Advisory Board, Nano Express.
- Dr. Satyavrata Samavedi has been selected as the Guest editor for Special issue of JoVE.
- Dr. Alan R Jacob has been invited as review editor in Frontiers of Physics as a specialist in soft matter physics.
- Dr. Kishalay Mitra inducted in the Editorial board of Materials and Manufacturing Processes, Taylor and Francis Journal, USA.
- Dr. Anand Mohan has been selected for the Editorial Board, Computer Research & Modeling.

#### **Research – Fellows and Committee Membership**

- Dr. Kirti Chandra Sahu has been elected as Fellow of the Indian Academy of Sciences (FASc).
- Dr. Chandra Shekhar Sharma has been selected as PAC Member, SERB SRG & NPDF Committee (Engineering Sciences) (2022-24).
- Dr. Kirti Chandra Sahu has been selected as Elected Fellow of Institute of Physics, UK.

#### **Research – Visiting Positions**

- Dr. Narasimha Mangadoddy has been selected as Visiting faculty at University of Cape Town.
- Dr. Satyavrata Samavedi has been selected as a Guest Researcher at NIMS, Japan.

#### Teaching

• Dr. Suhanya Duraiswamy (2023), Dr. Parag Pawar (2022) and Dr. Santhosh Kumar Devarai (2020) have been awarded with IIT Hyderabad Teaching excellence Award.

#### **Research Recognitions**

- Dr. Chandra Shekhar Sharma has been featured as one of the 75 under 50 scientists Shaping Today's India in a DST compendium as a part of Azadi ka Amrit Mahotsav Celebration of India's 75th year of Independence.
- Dr. Giridhar Madras has been awarded with the Research.com Chemistry in India Leader Award for being ranked in the top 10 scientists in India in chemistry.
- Dr. Kirti Chandra Sahu has been selected for the VASVIK Industrial Research for the Year 2021.
- Dr. Suhanya Duraiswamy has been awarded for the Best Poster presentation in International Research Conference on Microfluidics and Organ-On-A-Chip Technologies, Singapore.
- Dr. Chandra Shekhar Sharma, Dr. Giridhar Madras, Dr. Kirti Chandra Sahu, Dr. Kishalay Mitra, Dr. Narasimha Mangadoddy and Dr. Sunil Kumar Maity have been featured in Stanford University's ranking of the world's top 2% of scientists.
- Dr. Kishalay Mitra (2022), Dr Kirti Chandra Sahu (2021), Dr. Chandrasekhar Sharma (2020), have been awarded with IIT Hyderabad Research Excellence Award.
- Dr. Shelaka Gupta has been selected as one of the 75 Women in STEM to be featured in the second edition of She Is.
- Dr. Chandra Shekhar Sharma has been awarded with DST-Swarna Jayanti Fellowship in Engineering Sciences.















PHD STUDENTS

## Department of Chemical Engineering

#### Location:

Academic Block – A, IIT Hyderabad, IITH Main Road, Near NH-65, Sangareddy, Telangana, PIN 502284, INDIA

## Email:

head@che.iith.ac.in

office@che.iith.ac.in

Call:

+91 40 2301 6200



Scan this QR Code to visit the departmental website or go to https://che.iith.ac.in/



భారతీయ సాంకేతిక విజాన సంస్థ హైదరాబాద్ भारतीय प्रौद्योगिकी संस्थान हैदराबाद Indian Institute of Technology Hyderabad