Department of Chemical Engineering, IIT Bombay.

List of TAP, FA, and TA Ph.D Topics for Autum 2024-2025 (May 2024)

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Topic No	Email Address	Name of the faculty (email id)	Title:	Objectives (4-5 lines): You may provide a link to the additional information (Additional description, videos etc.) [Optional]	Area of the research (One key word)	Nature of the project (Experimental/Modeling/ Theoretical/):	Background required (e.g. Chemical Engg/Chemistry/Physics, Specific experimental expertise/Knowledge in coding, etc.):
TAP-1 (PW)	wangikar@iitb.ac.in	Pramod Wangikar	Development of genome-scale metabolic model (GEM) of Cupriavidus necator.	GEMs contain detailed information about all known biochemical reactions in a specific organism based on its genome and physiological information. GEMs can be simulated to gain meaningful insights about the organism and can aid in strain engineering and bioprocess development. While GEMs are now readily available for model organisms such as E. coli and yeast, significant more work is needed for non-model organisms. Cupriavidus necator is emerging as a new bacterial host for industrial bioproduction. C. necator has many interesting properties; it is chemolithotrophic, is capable of fixing CO2 and can use hydrogen as a source of energy. It can easily adapt between heterotrophic (using organic carbon such as sugar) and autotrophic (using inorganic carbon such as CO2) lifestyles. Here, we will develop, curate and simulate GEM for C. necator and combine it with spent media analysis, an experimental method based on LCMS to monitor hundreds of metabolites in the medium.	Metabolic modeling	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Eng. / Life Sciences
TAP-2 (PW)	wangikar@iitb.ac.in	Pramod Wangikar	Synthetic biology and metabolic engineering of fast-growing cyanobacteria.	Cyanobacteria or blue-green algae are a group of prokaryotes well known for their ability to carry out oxygenic photosynthesis. These photoautotrophs show greater photosynthetic efficiency, simpler genetic structures and faster growth compared to terrestrial plants and green algae. Moreover, cyanobacteria can be engineered genetically and can grow on non-arable land, waste-water and seawater. These properties make cyanobacteria an interesting host for biotechnological applications. In several proof-of-concept studies, cyanobacteria have been engineered to produce biofuels, plastics and commodity chemicals. However, a significant improvement in rate, yield and titer would be needed to make these processes commercially viable. In this project we propose to engineer a locally isolated strain of cyanobacteria, Synechococcus elongatus PCC11801 for the production of various platform chemicals. The work involves the following: (i) design and characterization of native and synthetic promoters, terminators and ribosomal binding sites and other DNA elements in cyanobacteria, (ii) development of synthetic biology tools for genome editing and transient gene expression in cyanobacteria, and (iii) engineering pathway of interest.	Synthetic biology	Experimental	Life sciences.
TAP-3 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Developing a framework for designing artificial tissue integrating reaction-diffusion and tissue mechanics models.	Living organisms start their life with a single cell, which divides multiple times to generate a number of cells. At the same time, a cascade of cellular signaling processes and gene regulatory networks set the gene expression pattern that leads to non-homogeneous mechanical properties of the tissue, ultimately guiding the final shape of functional organs. Motivated by this phenomena in living organisms, we would like to develop a framework for designing artificial tissues. On one hand, we will implement a generalized reaction-diffusion model in both two and three dimensions that will simulate any gene expression network. Parallely, to simulate the mechanical deformation of the tissue we utilize models of tissue mechanics such as vertex models representation . After successful implementation of both these models, we can make in-silico tissues that grow and change shape like real ones. This could help us design artificial tissues and implants that form specific shapes and functions on their own.	Tissue Mechanics; Systems Biology	Theoretical / Computational / Modelling	Interest in coding; No Bio background required (willingness to learn is enough)
TAP-4 (JA)	adhikari@iitb.ac.in	Jhumpa Adhikari	Molecular Simulation and Experimental Studies on Thermodynamics of High-Value Bio-chemicals derived from Biomass Valorization	https://sites.google.com/view/jhumpaadhikariiitb/openings	Biomass valorization	Both: Theoretical (Computational or Modelling) + Experimental	
TAP-5 (SD)	sonali.das@iitb.ac.in	Sonali Das	Catalyst and process development for sustainable conversion of Methane to C2 hydrocarbons.	Methane is a greenhouse gas that is often flared in current industrial practice. In light of the current climate change issues and changing energy landscape, the direct one-step conversion of methane to higher hydrocarbons using renewable energy sources is a much sought after goal. This project aims at the development of a new sustainable process and catalysts for the low temperature direct conversion of methane to higher hydrocarbons. The work will involve the synthesis and characterization of new nanostructured catalysts, lab-scale reactions and testing of developed catalysts, reaction kinetics, and operating parameter optimization. For more details, visit https://sites.google.com/view/das-lab/research	Catalysis & Reaction Engineering, Sustainability	Experimental	Chemical Engg./ Chemistry preferred
TAP-6 (SD)	sonali.das@iitb.ac.in	Sonali Das	Catalyst development for sustainable green hydrogen storage in liquid carriers	A rapid transition to the sustainable “hydrogen economy” is delayed by the lack of suitable hydrogen storage and transport systems. A potential way to safely store/ transport H2 is to store it in the form of a liquid hydrogen carrier (LHC) such as ammonia, which can be reversibly cycled by hydrogenation and dehydrogenation reactions to capture and release hydrogen. The success of ammonia-based LHC technology depends on the development of efficient ammonia decomposition technologies to release the green hydrogen. This project aims at the synthesis and development of new catalysts for low temperature cracking of ammonia to hydrogen and nitrogen by conventional thermal catalysis or by light-assisted photothermal catalysis. The work would entail development of new catalyst materials, detailed characterization, testing catalyst performance in reactors and detailed kinetic studies. [1]	Catalysis & Reaction Engineering, Sustainability	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engg. preferred

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TAP-7 (BKS)	bharat.k.suthar@iitb.ac.in	Bharatkumar Suthar	Advancing Li-ion Battery Technology: Characterization, Fast Charging, and Battery Management System for Packs	This PhD project relates to enhancing Li-ion battery technology through thorough cell characterization, efficient fast charging methods, and optimized battery management systems (BMS) for battery packs. The study aims to gain a deep understanding of cell behavior to improve fast charging efficiency while minimizing capacity fade. [2]	Battery management system	Both: Theoretical (Computational or Modelling) + Experimental	Chemical/Mechanical Engineering and Physics. Course Background: Transport, Computational Methods, Numerical Methods, Course Backgrond preferred but not mandatory: Electrochemical Systems, CRE Coding background: Python/Matlab/C/C++ will be preferred. However it is okay if you don't already have the background but one must have strong desire to learn these tools of scientific computing . Experimental background: 3 D printing preferred but not mandatory.
TAP-8 (RaD)	dasgupta.ratul@iitb.ac.in	Ratul Dasgupta	Prediction of wave breaking using ML algorithms - joint work with IITM and Microsoft Research	The work is theoretical and computational in nature to be done in collaboration with colleagues at Microsoft Research, Bangalore & Tel-Aviv and IIT Madras.	Surface waves	Theoretical / Computational / Modelling	Mechanical, Chemical (M.Tech. preferably) with strong academic performance. Good knowledge in programming with aptitude for physics and mathematics.
TAP-9 (YS)	yshastri@iitb.ac.in	Yogendra Shastri	Assessment of E-fuel production pathway using life cycle and techno-economic assessment	E-fuels are fuels produced from carbon di oxide captured using carbon capture techniques and green hydrogen. They are considered as promising replacements for conventional hydrocarbons. This project proposes to conduct early stage life cycle assessment and preliminary techno-economic assessment of selected E-fuels based on the processes developed by collaborating PSU. • Identify promising carbon capture, green hydrogen and E-fuel options • Quantify life cycle environmental impacts and economic feasibility of selected E-fuels and understand their trade-offs (if any) • Estimate potential greenhouse gas emission reduction at national scale through adoption of E-fuels • Propose process performance targets for achieving sustainability • Develop early stage technology ranking for further exploration	Sustainable energy	Theoretical / Computational / Modelling	Chemical Engineering, Biochemical Engineering, Biotechnology
Only those candidates who have external fellowsip/s like CSIR/DBT JRF can opt for the following topis [FA-1 (SBN) to FA-19 (AtM)]							
FA-1 (SBN)	noronha@iitb.ac.in	Santosh Noronha	Production of chiral pharma intermediates.	The objective of this project is to overproduce a key chiral pharma intermediate, currently extracted from plants. The strategies we propose to use include transferring pathways to microbial systems from plants and other microbial systems, manipulation of pathway fluxes in these systems, and engineering relevant enzymes to have improved catalytic activities.	Bioprocess engineering	Experimental	Project-related experience with biochemistry, microbiology and molecular biology techniques would be an advantage.
FA-2 (SBN)	noronha@iitb.ac.in	Santosh Noronha	Catalytic bioreactors	The objective is to design and implement catalytic bioreactors. Work elements will involve standardization of a catalytic system, characterization of kinetic and transport aspects, process optimization, and detection in real time.	Bioprocess engineering	Both: Theoretical (Computational or Modelling) + Experimental	Exposure to process reaction engineering or biocatalysis.
FA-3 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	An integrated model for organization of organoids and tumor spheroids in three dimensions.	The mechanism of organization of cells of different types to form a tissue in three dimensions is relevant in different biological contexts such as differentiation of cells into different cell types starting from stem cells and formation of tumors in the case of cancer. The two classes of model systems studied often in these contexts are organoids and tumor spheroids. Although these systems are studied extensively in two dimensional cell culture systems, three dimensional high resolution imaging methodologies are still developing. In this project, learning from the available 2D datasets and recently available 3D datasets, we will build an integrated model of three dimensional organization of tissue that will include systems biology aspect of tissue mechanics such as tissue proliferation, cell death, cellular signaling, as well as aspects of tissue mechanics such as actomyosin contractility and cell-cell adhesion. Altogether, using this computational framework, we plan to predict the organization of tissue in-vivo environment and guide future experiments.	Tissue Mechanics; Systems Biology	Theoretical / Computational / Modelling	Interest in coding; No Bio background required (willingness to learn is enough)

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FA-4 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Cell Division: an algorithm for packing spheres	Understanding packing of sphere-like particles in arbitrary dimensions is a long-standing problem of statistical physics. Most of the proposed algorithm starts from a dilute configuration and then either the particles are added one by one, the enclosing box compresses, or the particles grow. However, biological systems achieve this in a different way: duplication of the particle (i.e, cell division). In this project, we will ask how we can utilize this mechanism to generate packings with desired properties. We will implement a generalized algorithm that will achieve any target density in a given geometry starting from single or a small number of seeds. Furthermore, we will compare the packing efficiency and structural (dis)orders of the generated structures with those from the existing algorithms. Finally we will explore the effect of the confinement and aspect ratio in the generated packing. Successful implementation of this algorithm will open a new paradigm in the problem of packing of spheres and help us to model experimentally relevant packings of cells in confinements.	Soft Matter	Theoretical / Computational / Modelling	Programming
FA-5 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Effect of loop formation in dynamics of (bio)polymers	Formation of loops are ubiquitous in the context of biopolymers. For example, in the structure of chromatin, topologically associated domains (TAD) are often formed by cohesin mediated loop extrusion. The effect of loop formation in structure and dynamics of the chromatin is studied extensively using experimental data as well as numerical simulations. In this project, we will utilize the physics of flexible polymers to analytically study the effect of loop formation in the structure and dynamics of biopolymers. Moreover, from the trajectories of sparsely located points on a chromatin, we will formulate a Bayesian framework to predict whether a loop exists in a polymer and if it does, where the ends belong. Altogether, successful implementation of this approach will be an example of physics-assisted prediction of chromatin architecture from a dynamic dataset.	Polymer Physics	Theoretical / Computational / Modelling	Analytical and Programming Skills
FA-6 (SyD)	sayantan@che.iitb.ac.in	Sayantan Dutta and Abhijit Majumder	Computational and Experimental investigation of substrate-induced pattern formation of cell collectives	Utilizing biological and mechanical signaling, cells self-organize to specific patterns in different contexts spanning from cells in a living embryo to bacteria in a biofilm. On the other hand, substrates on which cells grow are known to influence the mechanical properties of the cell. In this project, we will explore how we can leverage a mechanical pattern on a substrate to induce patterns in the colonies of cells growing on it. We will begin with a computational model that will include cell-substrate interaction, cell-cell interaction, and tissue motility to understand the mechanism of substrate induced pattern formation in the collective of cells and robustly reproduce the experimental results from our in-house experiment (Prof. Majumder's lab) and literature. Next, we will leverage this model to explore the space of different mechanical patterns and to predict the induced pattern in the cell collectives. Finally, we will validate the model predictions using the experimental set-up.	Biological Pattern Formation; Cellular Mechanics	Both: Theoretical (Computational or Modelling) + Experimental	Interest to conduct both the computation and experiment.
FA-7 (SMe)	sarika@che.iitb.ac.in	Sarika Mehra	Upstream process development for recombinant therapeutics including MABs and vaccine subunits	https://www.eka.care/doctor/dr-vivek-h-lanje-cardiac-surgeon-nagpur/calendar/1-Consultation%20-REGULAR?cid=637ef7c5dbc983001e2c13bc	biochemical engineering	Both: Theoretical (Computational or Modelling) + Experimental	
FA-8 (SMe)	sarika@che.iitb.ac.in	Sarika Mehra	Synthetic Biology tools to create host cell lines for production of recombinant proteins		cell engineering	Experimental	background in molecular biology preferred
FA-9 (SMe)	sarika@che.iitb.ac.in	Sarika Mehra	Mathematical models for development of resistance in host			Theoretical / Computational / Modelling	
FA-10 (GAV)	ganeshav@iitb.ac.in	Ganesh Viswanathan	Countering cancer cell proliferation by enhancing cell death	Tilting the cancer cell fate from proliferation to cell-death is an emerging therapeutic paradigm. Tumor Necrosis Factor alpha (TNFa) is a pleiotropic cytokine involved in multiple phenotypic responses including cell survival and multiple modes of cell-death. The goal of this project is to understand TNFa induced cell-death and thereby identify approaches that enable the tilting of cellular response from proliferation to cell-death. To achieve this, the project will involve construction of a literature curated reaction network, development of discrete kinetic model, and performing systematic simulations .	Chemical Reaction Engineering	Theoretical / Computational / Modelling	Biotechnology, Chemical Engineering, Physics.
FA-11 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	An Autonomous Water Quality Monitoring and Water Treatment System for Waterbodies	We have been developing a complete water quality monitoring system consisting of a core module hosting an array of electrode/optical probe-based sensors for monitoring standard water-body parameters such as pH, temperature conductivity, turbidity, oxidation-reduction potential (ORP), dissolved oxygen (DO) etc., and reagent based quantification modules for specific chemical pollutants (e.g., fluoride - an inorganic pollutant, arsenic and chromium - metal pollutants etc.). Additional sensor modules can be installed to the core module, when required for a specific water body. The station is IOT enabled, and sensor readings are relayed to a wireless gateway at periodic intervals, which should be accessible anywhere in the world through a web interface. The entire system is envisaged to be locally powered at the deployment site, by a solar panel-battery combination, with uninterrupted operation over several weeks, without any manual intervention. One has to work in an interdisciplinary team and it will involve nanomaterials, 3D printing, nanomanufacturing and water sensors and water treatment as research areas.	Water Sensors and treatment	Experimental	(i) BTech/BE/MTech/ME in Chemical/Electrical/Mechanical/Materials Engg. or allied areas or, (ii) MSc in Physics/Chemistry/Electronics/Materials Sc. or allied areas

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FA-12 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	On the mechanism of nanoparticles in water disinfection: Using microfluidic devices to understand and design point of use systems	Disinfection by metal nanoparticle (NP) impregnated activated carbon (AC) is proposed in this project. This will be done in a gravity-driven filter-column set-up, which would run without any power, ideal in a resource-constrained scenario. Understanding the interaction between NPs and bacterial cells is thus crucial to explain the device performance. The project aims to uncover such biotic-abiotic interactions by microfluidic experiments, involving bacterial cell-laden water being flown, over PDMS gel casted or 3D printed channels (with different patterned surfaces), mimicking the intergranular pore structure of AC. The optimum hybrid material in terms of NP size and surface number density of these particles, on different patterned carbon surfaces would be found, to be used for the gravity-driven POU system. Thus, for the first time, experiments based on microfluidic platforms will result in development of a new engineering design of a power-free water disinfection system. The work will be as part of a team of other students with interdisciplinary background, with ample scope to learn and innovate. The research involves: (i) either designing and conducting experiments with microfluidic devices, or (ii) engineering of water treatment systems.	Microfluidics	Experimental	(i) MTech/ME/BTech/BE in Chemical/Mechanical/Environmental/Materials Engg. or allied Engg. branches or (ii) MSc in Microbiology/Life Sciences/Physics/Chemistry/Materials Sc. or allied basic science depts.
FA-13 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Anisotropic Nanoparticles: Synthesis, Mechanism and Applications	We have observed that, anisotropic nanoparticles, like nanorods, have higher chemical reaction rates than spherical or oval shaped (nearly spherical) nanoparticles. We hypothesize that, chemical reaction rate is a function of the shape of nanoparticles. In this project, one can do a combination of experiments and modeling/simulation or only experiments, to correlate nanoparticle shape with its reactivity. Simultaneously, one can work on its use for different ongoing applications in our laboratory.	Nanoparticles	Both: Theoretical (Computational or Modelling) + Experimental	ME/MTech/BE/BTech in Engineering (Chemical, Mechanical, Environmental, Materials) or MSc in Science (Physics, Chemistry, Materials)
FA-14 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth	Design of Additives to Control Dendritic Growth	Dendritic growth is a captivating phenomenon observed in various natural and synthetic systems, characterised by the formation of intricate, tree-like structures. In materials science, dendritic growth often occurs during solidification processes, where rapid cooling leads to the branching growth of crystalline structures. These dendrites exhibit a fascinating array of patterns and shapes, influenced by factors such as temperature gradients, impurities, and surface interactions. Understanding dendritic growth is crucial in fields ranging from metallurgy to biology, offering insights into complex phenomena such as pattern formation, fractal geometry, and the dynamics of phase transitions. This PhD topic will focus on the use of nanoparticle additives for tuning dendritic growth.	Solidification and pattern formation	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering, Physics, Physical Chemistry, Materials Science, Mechanical Engineering
FA-15 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth	Self Assembly of polyelectrolytes	Polyelectrolytes are macromolecules containing repeating units capable of dissociating in ionizing solvents, such as water. This process results in the formation of a highly charged polymeric chain composed of units bearing either positive or negative charges. Polyelectrolyte research is highly significant across biomedical engineering and environmental science. These charged polymers are pivotal in drug delivery systems, offering precise control over release kinetics by interacting with biological molecules and responding to environmental cues. Additionally, in wastewater treatment, polyelectrolytes aid in contaminant removal through flocculation and coagulation processes. Understanding polyelectrolyte behaviour is essential for developing sustainable solutions to global challenges in healthcare and environmental remediation. Polyelectrolytes show a remarkable ability to spontaneously organize into complex structures. This PhD position offers a unique chance to investigate the spontaneous organization and behaviour of charged polymers in solution. The selected PhD student will investigate the fundamental principles governing polyelectrolyte self-assembly and explore the influence of molecular architecture, charge density, and solvent conditions on assembly dynamics. The work will involve the use of advanced computational techniques.	self assembly and soft matter	Theoretical / Computational / Modelling	Chemical Engineering, Physics, Physical Chemistry, Materials Science, Mechanical Engineering
FA-16 (JS)	jrseth@gmail.com	Jyoti Seth and Abhijit Majumdar	Directed Cell Migration through substrate viscoelasticity	Directed cell migration plays a crucial role in physiological and pathological conditions. One important mechanical cue, known to influence cell migration, is the gradient of substrate elastic modulus (E). However, the cellular microenvironment is viscoelastic and hence the elastic property alone is not sufficient to define its material characteristics. In this topic, the student will develop our initial work on the migration of stem cells in response to the gradient of loss modulus. We will study the effect of mixed elastic and viscous modulus gradients and the influence of substrate deformation. This will be an opportunity for the student to build her/his apparatus for studying substrate cell response.	directed cell migration, gel rheology	Experimental	Chemical Engineering, Physical Chemistry, Microbiology, Biochemistry, etc.

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FA-17 (SRJ)	srjadhav@iitb.ac.in	Sameer Jadhav	Early cancer detection and cancer Treatment using electric fields (Electroporation)	The administration of anti-cancer drugs such as Cisplatin and Bleomycin is known to be significantly enhanced when used in conjunction with electroporation. Electroporation involves punching of holes of the size of few 10s of nanometers into bilayer membranes to put across polar drugs or nanoparticles. The long time and length scales associated with the pores merits a meso-scopic method such as Dissipative particle dynamics. With an exclusive aim to looking into a mechanism of membrane electroporation on mesoscopic length and time scales, we recently reported the dissipative particle dynamics (DPD) simulation results for systems with and without electrolytes. In this study, a polarizable DPD model of water is employed for accurate modelling of long range electrostatics near the water-lipid interfaces. The project will continue this work to simulate the interaction of nanoparticles with bilayer membranes under electric fields. The already available code will be further developed to simulate new scenarios and results will be compared with experiments. It is known that nanoparticles are effective in both early detection as well as delivery of anticancer agent. The dependence of the efficacy of delivery of these nanoparticles and their dependence on size and charge on the nanoparticles will be explored in this work. Both experiments and simulations will be performed References 1. Establishing an Electrostatics Paradigm for Membrane Electroporation in the Framework of Dissipative Particle DynamicsR Vaiwala, S Jadhav, R ThaokarJournal of chemical theory and computation 15 (10), 5737-5749, 2019 2. Electroporation using Dissipative Particle Dynamics with a novel protocol for applying Electric field R Vaiwala, S Jadhav, R Thaokar Journal of chemical theory and computation 15 (1), 603-612, 2018 3.Four-to-one coarse-grained polarisable water model for dissipative particle dynamics R Vaiwala, S Jadhav, R ThaokarMolecular Simulation 44 (7), 540-550,2018 4. Probing entropic repulsion through mesoscopic simulations R Vaiwala, R Thaokar EPL (Europhysics Letters) 120 (4), 48001, 2018 5.Electrostatic interactions in dissipative particle dynamics—Ewald-like formalism, error analysis, and pressure computation, R Vaiwala, S Jadhav, R ThaokarThe Journal of chemical physics 146 (12), 124904, 2017 6.Development of transmembrane potential in concentric spherical, confocal spheroidal, and bispherical vesicles subjected to nanosecond-pulse electric field S Nath, KP Sinha, RM Thaokar Physical Review E 101 (6), 062407, 2020 Supervisors: Prof. Sameer Jadhav and Prof. Rochish Thaokar	Molecular simulations	Theoretical / Computational / Modelling	Chemical engineering, chemistry
FA-18 (AtM)	amalani@iitb.ac.in	Ateeque Malani	Computational analysis of synthesis of porous materials	Several porous materials such as, metal organic frameworks (MOF), covalent organic frameworks (COF), zeolites, Hydrogen-bonded frameworks, are synthesized now a days. The basic principle is that a node molecule with Nx functionality (bond formation ability) reacts with linker of Ny functionality, resulting in an ordered porous structure. The porous characteristics (pore size, porosity, channel width, functional groups, etc) of these materials are controlled by choosing proper Node and linker molecules. However, the mechanism of formation, various stages during synthesis (pore formation, development and growth) are not known due to difficulty in probing. Hence, most of these synthesis are done on trial-and-error basis. The focus of this project is to to obtain molecular understanding of these process by computational modelling. (see https://doi.org/10.3390/separations6030033 and https://www.science.org/doi/full/10.1126/science.aal1585)	Reticular chemistry, MOF, COF, Zeolites	Theoretical / Computational / Modelling	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
FA-19 (AtM)	amalani@iitb.ac.in	Ateeque Malani	Modelling of early stages of cloud formation	The climate change is a reality which is creating extreme weather patterns of heavy rains and droughts which leads to loss of lives. The immediate reason is formation or absence of clouds in these events and hence understanding their formation is necessary. In this project, the focus is to probe early stages of formation of clouds in atmosphere by water condensation. Effects of various parameters would be explored.	Cloud formation, condensation, water adsorption	Theoretical / Computational / Modelling	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding

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List of TA topics that will be available for PhD students selected under TA cetegory in May 2024 admission round. All candidates who have applied under TA/RA/FA category are eligible to opt for TA choice.							
TA-A	picardo@iitb.ac.in	Jason R. Picardo	Pattern formation amid turbulence: how large-scale order survives small-scale chaos	The vast majority of flows in our daily experience are turbulent and yet we see patterns all around us. Ordered arrays of cloud streets, (turbulent) wind-driven waves with distinct wavelengths, and---for a more exotic example---Jupiter's red spot all testify to the ability of ordered patterns to arise and persist amidst turbulent fluctuations. In this project, we will specifically focus on understanding how patterns with length and time scales much greater than the turbulent flow arise and survive. We will do this in the specific context of waves driven by a tangential flow of turbulent air over the surface of a liquid layer. As we gain insight into this problem, we will be able to address other situations as well, and thereby attempt to uncover some general principles underlying pattern formation in turbulent flows. For more info on the project: https://www.che.iitb.ac.in/index.php/phd-ta-topic/pattern-formation-amid-turbulence-how-large-scale-order-survives-small-scale-chaos	fluid dynamics; instabilities	Theoretical / Computational / Modelling	This project will involve understanding and applying theories of pattern formation, stability analysis, and stochastic models of turbulence. Simulations will also be needed, but of simplified models, as the very nature of these problems precludes the use of direct numerical approaches. To get started, a knowledge of fluid dynamics, mathematics of ODEs and preferably also of PDEs is important. Experience using Matlab or Python is also useful. If you don't have a background in some of these areas, then don't worry---you can learn, but you must have a strong interest in them.
TA-B	picardo@iitb.ac.in	Jason R. Picardo; Partha Goswami	Multiscale CFD simulations of viscoelastic turbulence	This project aims to develop a state-of-the-art CFD code for predicting the turbulent flow of dilute polymer solutions. With this advanced computational tool, we will then explore two oustanding puzzles in the field of turbulent polymer solutions: (1) Elastic instabilities and the transition to elastic turbulence, and (2) drag reduction and its loss due to polymer breakage or scission. More information: https://www.che.iitb.ac.in/phd-ta-topic/multiscale-cfd-simulations-viscoelastic-turbulence	Turbulence; CFD	Theoretical / Computational / Modelling	The project relies heavily on fluid dynamics and numerical methods, and will involve coding in Fortran and Python. A good background in these areas will be very useful; if you dont have a background in some of these areas then you must have a strong interest to learn them.
TA-C	hnanavati@iitb.ac.in	Hemant Nanavati	Accurate Molecular Models for Real Polymers (TA/FA)	We develop useable, closed form, but accurate molecular models as well as elasticity relationships for real polymers, incorporating structural aspects. The applications include synthetic as well as high performance Bio-sourced polymers.	Polymer Physics, Statistical Themodynamics	Theoretical / Computational / Modelling	Chemical Engg/Chemistry/Physics
TA-D	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Elasticity of Spider Silk and Related Biopolymers	In this project, the aim is to understand quantitatively the molecular elasticity of biopolymers with potential engineering applications. The first example is Spider Dragline Silk, which may be several times stronger than steel (after normalizing the density). The work involves experimental, computational and theoretical analyses of the molecular structure of the biopolymer system. Work Aspects include: a) Microscopy, b) Molecular Simulations, c) Polymer Physics, d) Mathematical modelling, and e) Statistical Themodynamics	Biopolymer Physics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engg/Chemistry/Physics
TA-E	sharad_bhartiya@iitb.ac.in	Sharad Bhartiya	Behavioral systems theory based MPC	Dynamics systems are usually represented by transport type equations. Behavioral systems are based on a representation-free approach where the system behavior is manifested in terms of dynamic trajectories. This work will explore data enabled predictive control (DeePC)	Control theory	Theoretical / Computational / Modelling	control theory, math, coding
TA-F	sharad_bhartiya@iitb.ac.in	Sharad Bhartiya	Isolation of natural products: From elementary steps to production	Useful chemicals are available in natural products. However, separating the chemical of interest from the multicomponent mixture is difficult as the number of the "impurities" may run into hundreds. This work will explore chromatographic processes to accomplish the above. The work will entail understanding properties of adsorbents, solvents and attempt to build schema to go from these elementary steps to production level flowsheet.	Chromatographic Separations	Both: Theoretical (Computational or Modelling) + Experimental	Physical chemistry, chemical engineering, HPLC, GC, other characterization techniques
TA-G	wangikar@iitb.ac.in	Pramod Wangikar	Bioprocess optimization of CHO Cell cultures using Genome-scale metabolic models and spent media analysis.	Chinese hamster ovary (CHO) cell cultures are the platform of choice for biotherapeutic protein production. There is significant interest in using genome-scale metabolic models (GEM) to identify metabolic bottlenecks in protein production and to guide cell engineering and bioprocess optimization. Multiple versions of GEM for CHO cell line are available in literature and they are getting refined. Here we propose to combine GEM with spent media analysis, an experimental method based on LCMS to monitor hundreds of metabolites in the medium. The model will be simulated using the approach of dynamic flux balance analysis. The insights obtained will be used to optimize the bioprocess.	Metabolic modeling	Theoretical / Computational / Modelling	Chemical Engineering
TA-H	noronha@iitb.ac.in	Santosh Noronha	Production of chiral pharma intermediates.	The objective of this project is to overproduce a key chiral pharma intermediate, currently extracted from plants. The strategies we propose to use include transferring pathways to microbial systems from plants and other microbial systems, manipulation of pathway fluxes in these systems, and engineering relevant enzymes to have improved catalytic activities.	Bioprocess engineering	Experimental	Project-related experience with biochemistry, microbiology and molecular biology techniques would be an advantage.
TA-I	noronha@iitb.ac.in	Santosh Noronha	Catalytic bioreactors	The objective is to design and implement catalytic bioreactors. Work elements will involve standardization of a catalytic system, characterization of kinetic and transport aspects, process optimization, and detection in real time.	Bioprocess engineering	Both: Theoretical (Computational or Modelling) + Experimental	Exposure to process reaction engineering or biocatalysis.

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TA-J	sayantan.dutta@iitb.ac.in	Sayantan Dutta	An integrated model for organization of organoids and tumor spheroids in three dimensions.	The mechanism of organization of cells of different types to form a tissue in three dimensions is relevant in different biological contexts such as differentiation of cells into different cell types starting from stem cells and formation of tumors in the case of cancer. The two classes of model systems studied often in these contexts are organoids and tumor spheroids. Although these systems are studied extensively in two dimensional cell culture systems, three dimensional high resolution imaging methodologies are still developing. In this project, learning from the available 2D datasets and recently available 3D datasets, we will build an integrated model of three dimensional organization of tissue that will include systems biology aspect of tissue mechanics such as tissue proliferation, cell death, cellular signaling, as well as aspects of tissue mechanics such as actomyosin contractility and cell-cell adhesion. Altogether, using this computational framework, we plan to predict the organization of tissue in-vivo environment and guide future experiments.	Tissue Mechanics; Systems Biology	Theoretical / Computational / Modelling	Interest in coding; No Bio background required (willingness to learn is enough)
TA-K	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Cell Division: an algorithm for packing spheres	Understanding packing of sphere-like particles in arbitrary dimensions is a long-standing problem of statistical physics. Most of the proposed algorithm starts from a dilute configuration and then either the particles are added one by one, the enclosing box compresses, or the particles grow. However, biological systems achieve this in a different way: duplication of the particle (i.e, cell division). In this project, we will ask how we can utilize this mechanism to generate packings with desired properties. We will implement a generalized algorithm that will achieve any target density in a given geometry starting from single or a small number of seeds. Furthermore, we will compare the packing efficiency and structural (dis)orders of the generated structures with those from the existing algorithms. Finally we will explore the effect of the confinement and aspect ratio in the generated packing. Successful implementation of this algorithm will open a new paradigm in the problem of packing of spheres and help us to model experimentally relevant packings of cells in confinements.	Soft Matter	Theoretical / Computational / Modelling	Programming
TA-L	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Effect of loop formation in dynamics of (bio)polymers	Formation of loops are ubiquitous in the context of biopolymers. For example, in the structure of chromatin, topologically associated domains (TAD) are often formed by cohesin mediated loop extrusion. The effect of loop formation in structure and dynamics of the chromatin is studied extensively using experimental data as well as numerical simulations. In this project, we will utilize the physics of flexible polymers to analytically study the effect of loop formation in the structure and dynamics of biopolymers. Moreover, from the trajectories of sparsely located points on a chromatin, we will formulate a Bayesian framework to predict whether a loop exists in a polymer and if it does, where the ends belong. Altogether, successful implementation of this approach will be an example of physics-assisted prediction of chromatin architecture from a dynamic dataset.	Polymer Physics	Theoretical / Computational / Modelling	Analytical and Programming Skills
TA-M	sayantan@che.iitb.ac.in	Sayantan Dutta and Abhijit Majumder	Computational and Experimental investigation of substrate-induced pattern formation of cell collectives	Utilizing biological and mechanical signaling, cells self-organize to specific patterns in different contexts spanning from cells in a living embryo to bacteria in a biofilm. On the other hand, substrates on which cells grow are known to influence the mechanical properties of the cell. In this project, we will explore how we can leverage a mechanical pattern on a substrate to induce patterns in the colonies of cells growing on it. We will begin with a computational model that will include cell-substrate interaction, cell-cell interaction, and tissue motility to understand the mechanism of substrate induced pattern formation in the collective of cells and robustly reproduce the experimental results from our in-house experiment (Prof. Majumder's lab) and literature. Next, we will leverage this model to explore the space of different mechanical patterns and to predict the induced pattern in the cell collectives. Finally, we will validate the model predictions using the experimental set-up.	Biological Pattern Formation; Cellular Mechanics	Both: Theoretical (Computational or Modelling) + Experimental	Interest to conduct both the computation and experiment.
TA-N	adhikari@iitb.ac.in	Jhumpa Adhikari	Predicting & Understanding Thermophysical Properties of Phase Change Materials via Molecular Simulations	A reversible phase transition (e.g. solid-solid, solid-liquid, liquid-vapour) involves latent heat at the transition temperature for a given pressure. In this project we will be performing molecular simulations to predict the thermophysical properties of novel materials for use in thermal energy storage and understand the underlying molecular level interactions occurring in the different phases. For more information, please email at adhikari@che.iitb.ac.in	Phase change materials	Theoretical / Computational / Modelling	
TA-O	swaticb@che.iitb.ac.in	Swati Bhattacharya	Computational study of the human anti-HIV protein SAMHD1 and VpX, a virion-associated protein of Human Immunodeficiency Virus 2 (HIV-2).	We are a computational biophysics research group and our primary focus is on understanding disease and immunity at a molecular level. This is done with the help of molecular dynamics simulations, machine learning tools and other computational techniques that help us understand how molecules such as proteins interact with each other. The insights can pave the way for the discovery of new drugs. Our primary focus is on HIV and the proteins of interest are SAMHD1, which is a human protein that prevents HIV-1 infection and VpX which is a viral protein that counters SAMHD1, i.e promotes infection. We will study the interactions between the two proteins and try to identify small molecules that can disrupt the interactions, i.e can be potential therapeutics for HIV. https: //sites.google.com/view/swatibhattacharya/home	Health and Life Sciences, Molecular Simulations, Thermodynamics, Computational biology	Theoretical / Computational / Modelling	Motivated individuals with a background in Chemical Engg/Chemistry/Physics/Biotech are welcome. An interest in coding and computational modelling is required. The student is expected to learn various computational tools.

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TA-P	swaticb@che.iitb.ac.in	Swati Bhattacharya	Modeling and Simulations of Sorcin, a protein associated with multi drug resistant cancers.	Sorcin is a calcium binding oncoprotein expressed at high levels in several human tumors such as leukemia, gastric, breast and ovarian cancers. Sorcin is an essential oncoprotein and there is growing evidence for its role in multi-drug resistant cancers. Our goal is to uncover its working through molecular simulations, understand its role in MDR cancers and attempt to find a druggable way to toggle its activity. The project will involve the study of the protein through all atom molecular simulations, machine learning tools and other computational methods. We are a computational biophysics research group and our primary focus is on understanding disease and immunity at a molecular level. This is done with the help of molecular dynamics simulations and other computational techniques that help us understand how molecules such as proteins interact with each other. The insights can pave the way for the discovery of new drugs. https://sites.google.com/view/swatibhattacharya/home	Computational biology, thermodynamics	Theoretical / Computational / Modelling	Motivated individuals with a background in Chemical Engg/Chemistry/Physics/Biotech are welcome. An interest in coding and computational modelling is required. The student is expected to learn various computational tools.
TA-Q	amol.subhedar@iitb.ac.in	Amol Subhedar	Development of a ternary lattice Boltzmann model to study double emulsions in micro-channels	Double emulsions, complex systems with unique properties and promising applications, are gaining considerable attention. One significant challenge in understanding them lies in accurately modeling the dynamics of triple junctions. To address this, we suggest employing a lattice Boltzmann model, particularly the color gradient variant tailored for three-phase flow. We plan to evaluate the model's accuracy using multi-scale expansions and then utilize it to investigate formation of double emulsions in a mircochannel.	Computational fluid dynamics	Theoretical / Computational / Modelling	
TA-R	amol.subhedar@iitb.ac.in	Amol Subhedar	Galilean Invariant model for multi-phase suspensions	computational study of suspensions involves tracking solid particles in a two-phase flow system. In the case of moving solid bodies in a single-phase flow, particle-based solvers (like the lattice Boltzmann method) treat the solid body as an effective fluid medium with high viscosity. The situation is slightly more involved with two fluid phases as it requires a prescription for a wetting boundary condition at the triple junction (in this case, where two fluid and one solid phase meet). The challenge here is ensuring that the no-slip and wetting boundary conditions are satisfied at the exact location inside the diffuse interface.	Computatonal fluid dynamics	Theoretical / Computational / Modelling	
TA-S	picardo21@gmail.com	Amol Subhedar, Jason Picardo	2. Thermofluid dynamics of melt-water in and under glaciers (Glacial fluid mechanics)	The Himalayan glaciers are a source of fresh water for millions. So the possibility of them retreating, given the accelerated pace of climate change, is a dire one. Moreover, the melting of the glaciers could translate into a rise in flash floods. Predicting the behaviour of glaciers, however, is a difficult task, due to a dearth of data (although recent campaigns have been launched to remedy this) and a lack of fundamental understanding of the mechanics of glacial flows. This project seeks to address the latter issue and investigate the flow in and of glaciers, with an emphasis on identifying the fundamental mechanisms at work. For more information please visit: https://www.che.iitb.ac.in/phd-ta-topic/glaciers-dynamics-melting-and-flow	Glacial fluid mechanics	Theoretical / Computational / Modelling	This project will require the development and analysis of mathematical models, which account for the coupling between the mechanics of flow and the thermodynamics of melting. The project relies heavily on fluid dynamics, math related to PDEs, and numerical methods, and will involve coding. A good background in these areas will be very useful; if you dont have a background in some of these areas then you must have a strong interest to learn them.
TA-T	mbhushan@iitb.ac.in	Mani Bhushan	Sensor placement and scheduling for accurate state and parameter estimation in distributed parameter systems using Gaussian process modeling	Gaussian process modeling has emerged as a popular data driven approach to model spatial and temporal variability in a process. In state estimation for distributed parameter systems, estimation errors vary across space as well as time. Most estimation approaches assume these errors to be Gaussian. Under this assumption, the estimation errors can be modeled as a Gaussian process. Various measures available in literature for characterizing information content in Gaussian processes can be then exploited to simultaneously identify optimal location of sensors as well as optimal schedule of sensing.	State estimation and sensor placement	Theoretical / Computational / Modelling	Good aptitude for maths/stochastics, comfort/interest in coding
TA-U	mbhushan@iitb.ac.in	Mani Bhushan	Online update of data driven models using state estimation approaches	In the current age of artificial intelligence and machine learning, data driven models are widely being used to model various processes. The dynamic behaviour of any system (such as a chemical manufacturing process) changes with time due to various events such as failures, upgrades, process modifications, etc. In such situations, updating data driven models to accurately represent the true process becomes challenging since these models have a large number of parameters and also often only a limited set of measurements is available in the plant. In this work, we plan to investigate state and parameter estimation ideas to update parameters of such models. Dimensionality reduction approaches will also be investigated to reduce the size of the problem.	Machine learning and State estimation	Theoretical / Computational / Modelling	Good aptitude for maths/stochastics, comfort/interest in coding
TA-V	mbhushan@iitb.ac.in	Mani Bhushan	Use of Large Language Models to automate generation of a database of pollution sources	Variety of LLMs are being widely used in various domains to scan existing literature/documents to answer meaningful questions. In this work, we propose to use existing LLMs to generate of a database of pollution sources in the Indian subcontinent as reported in literature. Besides text processing, this work will also involve use of image processing tools.	Machine learning	Theoretical / Computational / Modelling	Good aptitude for maths/stochastics, comfort/interest in coding

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TA-W	bharat.k.suthar@gmail.com	Prof. Bharatkumar Suthar, Prof Jason Picardo	Multiscale Modeling and Simulation of Battery Pack for E-mobility and Drone Application	With the rising popularity of electric vehicles (EVs) and drones, ensuring the efficiency and safety of battery packs is paramount. This PhD research aims to enhance battery pack design through multiscale modeling and simulation techniques, focusing on improving thermal management strategies. By integrating Battery Pack Simulations and Computational Fluid Dynamics (CFD), the study seeks to gain deep insights into pack behavior, including heat generation and dissipation. Additional goal of this project is the derivation of reduced order model (effective medium theory) for real time prediction and optimization of battery pack performance. Through this research, we aim to tackle challenges such as thermal runaway mitigation and optimizing operating conditions. By bridging the gap between microscale battery cell dynamics and macroscopic pack behavior, we can develop more effective strategies for cooling and heat management.	Thermal management of battery pack	Theoretical / Computational / Modelling	Chemical/Mechanical Engineering and Physics. Course Background: Transport, Computational Methods, Numerical Methods, Course Backgrond preferred but not mandatory: Electrochemical Systems, CRE Coding background: Python/Matlab/C/C++ will be preferred. However it is okay if you don't already have the background but one must have strong desire to learn these tools of scientific computing .
TA-X	bharat.k.suthar@iitb.ac.in	Bharatkumar Suthar	Na-ion Battery Dynamics: Modeling, Validation, and Capacity Fade Analysis	This PhD research relates to Na-ion battery technology, focusing on building accurate models, validating them through experiments, and understanding capacity fade. Given India's increasing energy needs and the push for sustainable solutions, Na-ion batteries hold promise for the country's energy future. A key part of this research is figuring out why Na-ion batteries lose capacity over time. By understanding this, the study hopes to find ways to make these batteries last longer, which could be crucial for India's energy goals.	Battery Modeling and Design	Both: Theoretical (Computational or Modelling) + Experimental	Chemical/Mechanical Engineering and Physics. Course Background: Transport, Computational Methods, Numerical Methods, Course Backgrond preferred but not mandatory: Electrochemical Systems, CRE Coding background: Python/Matlab/C/C++ will be preferred. However it is okay if you don't already have the background but one must have strong desire to learn these tools of scientific computing . Experimental background: 3 D printing preferred but not mandatory.
TA-Y	dasgupta.ratul@iitb.ac.in	Ratul Dasgupta	Theory of simulations of jets in Faraday waves - collaborative work with Univ. Bordeaux, France	The work aims at understanding the secondary instabilities which are responsible for the emergence of spray from the Faraday instability. The work is in collaboration with Prof. Sakir Amiroudine at Univ. Bordeaux.		Theoretical / Computational / Modelling	Chemical, Mechanical Engg. (preferably students with an M.Tech degree). Strong in physics and mathematics with an interest in programming.
TA-Z	jogwar@iitb.ac.in	Sujit Jogwar	Electrification of integrated and intensified processes	Decarbonization and use of renewable electricity are key drivers for sustainable practices for the future chemical industries. This project aims at assessing the impact of electrification on (thermally) integrated and intensified processes and transforming them to meet the demands of the future.	Sustainability	Theoretical / Computational / Modelling	
TA-AA	jogwar@iitb.ac.in	Sujit Jogwar	Data-driven distributed estimation and control of chemical processes	Distributed estimation and control has emerged as a natural paradigm for efficient operation of integrated processes. This project aims at developing data-driven approaches for estimation and control of chemical processes in the context of distributed computing.	Process Systems Engineering	Theoretical / Computational / Modelling	
TA-AB	sarika@che.iitb.ac.in	Sarika Mehra	Upstream process development for recombinant therapeutics including MABs and vaccine subunits	https://www.eka.care/doctor/dr-vivek-h-lanje-cardiac-surgeon-nagpur/calendar/1-Consultation%20-REGULAR?cid=637ef7c5dbc983001e2c13bc	biochemical engineering	Both: Theoretical (Computational or Modelling) + Experimental	
TA-AC	sarika@che.iitb.ac.in	Sarika Mehra	Synthetic Biology tools to create host cell lines for production of recombinant proteins		cell engineering	Experimental	background in molecular biology preferred
TA-AD	sarika@che.iitb.ac.in	Sarika Mehra	Mathematical models for development of resistance in host			Theoretical / Computational / Modelling	
TA-AE	ganeshav@iitb.ac.in	Ganesh Viswanathan	Countering cancer cell proliferation by enhancing cell death	Tilting the cancer cell fate from proliferation to cell-death is an emerging therapeutic paradigm. Tumor Necrosis Factor alpha (TNFa) is a pleiotropic cytokine involved in multiple phenotypic responses including cell survival and multiple modes of cell-death. The goal of this project is to understand TNFa induced cell-death and thereby identify approaches that enable the tilting of cellular response from proliferation to cell-death. To achieve this, the project will involve construction of a literature curated reaction network, development of discrete kinetic model, and performing systematic simulations .	Chemical Reaction Engineering	Theoretical / Computational / Modelling	Biotechnology, Chemical Engineering, Physics.

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TA-AF	jyotiseth@iitb.ac.in	Jyoti R Seth	Design of Additives to Control Dendritic Growth	Dendritic growth is a captivating phenomenon observed in various natural and synthetic systems, characterised by the formation of intricate, tree-like structures. In materials science, dendritic growth often occurs during solidification processes, where rapid cooling leads to the branching growth of crystalline structures. These dendrites exhibit a fascinating array of patterns and shapes, influenced by factors such as temperature gradients, impurities, and surface interactions. Understanding dendritic growth is crucial in fields ranging from metallurgy to biology, offering insights into complex phenomena such as pattern formation, fractal geometry, and the dynamics of phase transitions. This PhD topic will focus on the use of nanoparticle additives for tuning dendritic growth.	Solidification and pattern formation	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering, Physics, Physical Chemistry, Materials Science, Mechanical Engineering
TA-AG	jyotiseth@iitb.ac.in	Jyoti R Seth	Self Assembly of polyelectrolytes	Polyelectrolytes are macromolecules containing repeating units capable of dissociating in ionizing solvents, such as water. This process results in the formation of a highly charged polymeric chain composed of units bearing either positive or negative charges. Polyelectrolyte research is highly significant across biomedical engineering and environmental science. These charged polymers are pivotal in drug delivery systems, offering precise control over release kinetics by interacting with biological molecules and responding to environmental cues. Additionally, in wastewater treatment, polyelectrolytes aid in contaminant removal through flocculation and coagulation processes. Understanding polyelectrolyte behaviour is essential for developing sustainable solutions to global challenges in healthcare and environmental remediation. Polyelectrolytes show a remarkable ability to spontaneously organize into complex structures. This PhD position offers a unique chance to investigate the spontaneous organization and behaviour of charged polymers in solution. The selected PhD student will investigate the fundamental principles governing polyelectrolyte self-assembly and explore the influence of molecular architecture, charge density, and solvent conditions on assembly dynamics. The work will involve the use of advanced computational techniques.	self assembly and soft matter	Theoretical / Computational / Modelling	Chemical Engineering, Physics, Physical Chemistry, Materials Science, Mechanical Engineering
TA-AH	psg@iitb.ac.in	Partha Sarathi Goswami	Investigation on clustering of micro particles/droplets in wall bounded turbulent flows using CFD and experiments	The objective of the project is to investigate the interaction between particle and turbulence and characterising the clustering of the particles using direct numerical simulations (DNS) and PIV experiments. An in-house or Open source code will be used for DNS.	CFD and EFD (PIV)	Both: Theoretical (Computational or Modelling) + Experimental	Chemical/Mechanical Engineering, Physics
TA-AI	psg@iitb.ac.in	Partha Sarathi Goswami	Direct Numerical Simulations (DNS) to investigate the effect of inertial particles on structures and regeneration cycle of fluid turbulence under external field.	In this project we want to investigate the effect of particles on the structure of fluid turbulence and the generation of fluid phase turbulence.	CFD (DNS)	Theoretical / Computational / Modelling	Chemical/Mechanical Engineering, Physics
TA-AJ	psg@iitb.ac.in	Partha Sarathi Goswami	Dynamics of cohesive spherical and non spherical particles in spouted and spout-fluid bed	Experimental investigation on dynamics, mixing and segregation of Cohesive powder in spouted bed. CFD computation will also be performed and results will be compared with the experiments	Fluidization and Spouting	Both: Theoretical (Computational or Modelling) + Experimental	Chemical/Mechanical Engineering, Physics
TA-AK	srjadhav@iitb.ac.in	Sameer Jadhav	Flow analysis and control in microfluidic networks	Microfluidics technology has been seen to have great potential in lab-on-a-chip applications including chemical analysis and diagnostics. However, flow control in these networks requires either a pneumatic or fluidic control layer over the microfluidic layer. Recent studies have shown that integrated flow control may be achieved by introducing capacitive elements or obstacles in the flow path so that system response becomes non-linear as required for flow switching. In this project we explore several designs and optimize geometric and flow parameters of the microfluidic network for desired flow control. We intend to use Ansys® and OpenFOAM® (open source CFD software) for this project.	Computational fluid dynamics	Theoretical / Computational / Modelling	Chemical engineering, mechanical engineering

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TA-AL	srjadhav@iitb.ac.in	Sameer Jadhav	Early cancer detection and cancer Treatment using electric fields (Electroporation)	The administration of anti-cancer drugs such as Cisplatin and Bleomycin is known to be significantly enhanced when used in conjunction with electroporation. Electroporation involves punching of holes of the size of few 10s of nanometers into bilayer membranes to put across polar drugs or nanoparticles. The long time and length scales associated with the pores merits a meso-scopic method such as Dissipative particle dynamics. With an exclusive aim to looking into a mechanism of membrane electroporation on mesoscopic length and time scales, we recently reported the dissipative particle dynamics (DPD) simulation results for systems with and without electrolytes. In this study, a polarizable DPD model of water is employed for accurate modelling of long range electrostatics near the water-lipid interfaces. The project will continue this work to simulate the interaction of nanoparticles with bilayer membranes under electric fields. The already available code will be further developed to simulate new scenarios and results will be compared with experiments. It is known that nanoparticles are effective in both early detection as well as delivery of anticancer agent. The dependence of the efficacy of delivery of these nanoparticles and their dependence on size and charge on the nanoparticles will be explored in this work. Both experiments and simulations will be performed References 1. Establishing an Electrostatics Paradigm for Membrane Electroporation in the Framework of Dissipative Particle DynamicsR Vaiwala, S Jadhav, R ThaokarJournal of chemical theory and computation 15 (10), 5737-5749, 2019 2. Electroporation using Dissipative Particle Dynamics with a novel protocol for applying Electric field R Vaiwala, S Jadhav, R Thaokar Journal of chemical theory and computation 15 (1), 603-612, 2018 3.Four-to-one coarse-grained polarisable water model for dissipative particle dynamics R Vaiwala, S Jadhav, R ThaokarMolecular Simulation 44 (7), 540-550,2018 4. Probing entropic repulsion through mesoscopic simulations R Vaiwala, R Thaokar EPL (Europhysics Letters) 120 (4), 48001, 2018 5.Electrostatic interactions in dissipative particle dynamics—Ewald-like formalism, error analysis, and pressure computation, R Vaiwala, S Jadhav, R ThaokarThe Journal of chemical physics 146 (12), 124904, 2017 6.Development of transmembrane potential in concentric spherical, confocal spheroidal, and bispherical vesicles subjected to nanosecond-pulse electric field S Nath, KP Sinha, RM Thaokar Physical Review E 101 (6), 062407, 2020 Supervisors: Prof. Sameer Jadhav and Prof. Rochish Thaokar	Molecular simulations	Theoretical / Computational / Modelling	Chemical engineering, chemistry
TA-AM	jrseth@gmail.com	Jyoti Seth and Abhijit Majumdar	Directed Cell Migration through substrate viscoelasticity	Directed cell migration plays a crucial role in physiological and pathological conditions. One important mechanical cue, known to influence cell migration, is the gradient of substrate elastic modulus (E). However, the cellular microenvironment is viscoelastic and hence the elastic property alone is not sufficient to define its material characteristics. In this topic, the student will develop our initial work on the migration of stem cells in response to the gradient of loss modulus. We will study the effect of mixed elastic and viscous modulus gradients and the influence of substrate deformation. This will be an opportunity for the student to build her/his apparatus for studying substrate cell response.	directed cell migration, gel rheology	Experimental	Chemical Engineering, Physical Chemistry, Microbiology, Biochemistry, etc.
TA-AN	amalani@iitb.ac.in	Ateeque Malani	Computational analysis of synthesis of porous materials	Several porous materials such as, metal organic frameworks (MOF), covalent organic frameworks (COF), zeolites, Hydrogen-bonded frameworks, are synthesized now a days. The basic principle is that a node molecule with Nx functionality (bond formation ability) reacts with linker of Ny functionality, resulting in an ordered porous structure. The porous characteristics (pore size, porosity, channel width, functional groups, etc) of these materials are controlled by choosing proper Node and linker molecules. However, the mechanism of formation, various stages during synthesis (pore formation, development and growth) are not known due to difficulty in probing. Hence, most of these synthesis are done on trial-and-error basis. The focus of this project is to to obtain molecular understanding of these process by computational modelling. (see https://doi.org/10.3390/separations6030033 and https://www.science.org/doi/full/10.1126/science.aal1585)	Reticular chemistry, MOF, COF, Zeolites	Theoretical / Computational / Modelling	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
TA-AO	amalani@iitb.ac.in	Ateeque Malani	Modelling of early stages of cloud formation	The climate change is a reality which is creating extreme weather patterns of heavy rains and droughts which leads to loss of lives. The immediate reason is formation or absence of clouds in these events and hence understanding their formation is necessary. In this project, the focus is to probe early stages of formation of clouds in atmosphere by water condensation. Effects of various parameters would be explored.	Cloud formation, condensation, water adsorption	Theoretical / Computational / Modelling	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
TA-AP	sanjaym@iitb.ac.in	Sanjay Mahajani	Catalysis and Process development for Green Chemicals	The work involves synthesis, characterization and performance evaluation of solid catalysts for industrially important chemicals made from renewable feedstock meeting the requirement of sustainable goals. Kinetic model will be developed to design the reactor on commercial scale. Student, if interested, will also work on computational catalysis, and process simulations for techno-economic and life cycle assessment.			

Department of Chemical Engineering, IIT Bombay.

List of TAP, FA, and TA Ph.D Topics for Autum 2024-2025 (May 2024)

You have to submit your preferences based on the following topics on or before 30-Apr-2024 in the google form shared in the departmental (Chemical Engineering) website

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TA-AQ	sanjaym@iitb.ac.in	Sanjay Mahajani	Foundry sand reclamation towards circular economy	The work involves technology development for thermal and chemical reclamation of waste foundry sand. A proof of concept will be established in laboratory and taken forward towards pilot and commercial scales. Techno-economic and life cycle assessment for the proposed solution would be carried to assess its sustainability potential.			
TA-AS	ravigudi@iitb.ac.in	Ravi Gudi and Sharad Bhartiya	AI & ML based product discovery and development	The project is computational in nature, and will focus on leveraging advances in AI & ML towards product discovery and its development, as applied to problems in healthcare, energy materials and environmental applications. Based on the incorporation of first principles knowledge of thermodynamics, molecular simulations and measured macroscopic properties, into AI & ML based knowledge representation approaches, the project will seek to build structure property relationships that will help in product discovery and development. The project is a continuation of an ongoing PhD work in the area of physics inspired neural networks.			
TA-AT	ravigudi@iitb.ac.in	Ravi Gudi	Understanding and modelling multi-scale interactions for ecological footprint assessment in manufacturing plants: Towards sustainable production practices	The escalating concerns surrounding environmental degradation and resource depletion necessitate a comprehensive evaluation of manufacturing processes. This topic focuses on the complex interplay between production activities and their environmental impacts. Employing a multidisciplinary approach, the study will utilize life cycle assessment, carbon footprint analysis, water footprint assessment, and other relevant methodologies to quantify and analyze the ecological footprints of manufacturing operations. And further develop various sustainability interventions and technological advancements in reducing ecological footprints while maintaining or enhancing production efficiency through optimization approaches.			
TA-AU	madhu@che.iitb.ac.in	Madhu Vinjamur	Enhanced Diffusion-based Loading of Drugs on Mesoporous Silica from Supercritical Carbon dioxide	The use of mesoporous nanoparticles (MSPs) as carriers for drug delivery systems has gained importance, as they are now recognized as GRAS (Generally Recognized as Safe) for human intake. MSPs have a porous structure varying from 2-50 nm. These pores provide a high surface area for adsorption of drug, yielding high loadings due to their high surface area to volume ratios. However diffusional resistance of the solid drug to the pore surface often poses a problem. Recently DiSupLo (Diffusion Supported Loading) method using ethanol vapors was reported for fast, uniform and controlled drug loading on MSPs. However, at the end of the process ethanol requires removal from the solid mixture of the drug and MSPs through drying, which may clog the pores hindering release of the loaded drug from the pores. Moreover, ethanol may not be a suitable solvent for the drug. On the contrary, Supercritical carbon dioxide (scCO2) is known to solubilize a wide variety of drugs. It is GRAS and a green substitute to the traditional organic solvents. Moreover, removal of scCO2 at the end of the operation simply requires depressurization of the vessel. The present work will explore a new method: “Supercritically Enhanced Diffusion-based Loading” on MSPs by replacing ethanol with scCO2 for carrying the drug to MSP as the two would be uniformly homogenized as a solid mixture. There would be several advantages of the process, as diffusional resistance of the drug transfer to the bed heights of the porous MSPs would be minimized enabling uniform, fast, and efficient loading, thereby less amount of drug would be needed for making the drug formulation with MSPs of the desired loading having uniform concentration.			