Department of Chemical Engineering, IIT Bombay.

List of TAP, FA, and TA Ph.D Topics for Spring 2024-2025 (Dec 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.):
List of TAP topics available for PhD candidates to be admitted.							
TAP-1 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Computational Biophysical modelling for Designing Artificial Tissues.	Living organisms start their life with a single cell, which divides multiple times to generate a number of cells. At the same time, chemical patterns establish in the cells leading 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 computational 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 computational 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.	Biophysical Modeling	Theoretical / Computational / Modelling	Engineering/Physics/Physical Chemistry; Interest in Coding
TAP-2 (SyD)	sayantan.dutta@iitb.ac.in	Mithun Chowdhury (MEMS) and Sayantan Dutta	Self Propulsion of Chemically Active Droplets under Surface Tension	Microscopic active droplets can swim on their own in viscous fluids due to solute exchanges with the surrounding fluid and resulting interfacial flows. Unlike asymmetric active colloids, these isotropic droplets use nonlinear solute transport and Marangoni flows for spontaneous movement. This interaction also leads to complex individual and collective behaviors. Their simple design and sensitivity to physical and chemical signals make them intriguing for researchers in physics, chemistry, biology, and fluid dynamics, who study self-propulsion, develop synthetic cellular models, or explore biomedical and engineering applications. In the proposed work we will use a structured surfactant bath to see self-propulsion of liquid crystal droplets by simple optical microscopy measurements. Further we will develop analytical and computational models to establish physical principles governing it.	Active Matter	Both: Theoretical (Computational or Modelling) + Experimental	Engineering, Physics, Physical Chemistry
TAP-3 (PW)	wangikar@iitb.ac.in	Pramod Wangikar	Metabolic Pathway Optimization for Enhanced Exopolysaccharide (EPS) Production in Cyanobacteria: A Systems Biology Approach	This research seeks to uncover and optimize the metabolic pathways responsible for high-rate exopolysaccharide (EPS) production in Anabaena 33047, a cyanobacterial strain with potential applications in sustainable biomanufacturing. By employing a systems biology framework, we will analyze gene expression, metabolic flux distributions, and regulatory networks integral to EPS biosynthesis. A combination of targeted and untargeted metabolomics, using LC-MS, will be used to map intracellular and extracellular metabolite concentrations, identifying pathway bottlenecks and congestion points. Furthermore, 13C isotope-assisted Metabolic Flux Analysis (INST-MFA) will trace carbon fluxes through essential pathways, including the Calvin cycle, glycolysis, and the TCA cycle, under varying growth and EPS-producing conditions. By integrating multi-omics data with the genome-scale model iAnC892, constrained using transcriptional and 13C-MFA data, we aim to simulate and redesign metabolic fluxes. In collaboration with Prof. Suvarn Kulkarni of Chemistry Department and Prof. Yinjie Tang and Prof. Himadri Pakrasi at Washington University in St. Louis, this project will identify novel targets for genetic modification to enhance EPS yield and tailor product structure for specific industrial uses. The outcomes will contribute foundational insights to cyanobacterial metabolic engineering for bioresource optimization.	Biotechnology	Both: Theoretical (Computational or Modelling) + Experimental	Biotechnology; Life Sciences.
TAP-4 (PW)	wangikar@iitb.ac.in	Pramod Wangikar	Elucidating the Structural Determinants of Exopolysaccharide (EPS) Mechanical Properties in Anabaena 33047 for Biomaterial Applications	This PhD research project focuses on characterizing the chemical and structural composition of exopolysaccharides (EPS) produced by Anabaena 33047 and evaluating how these structural features affect the mechanical properties of EPS-derived fibers. Working in collaboration with Prof. Suvarn Kulkarni of Chemistry Dept and Prof. Yinjie Tang, and Prof. Himadri Pakrasi at Washington University in St. Louis, this study will analyze EPS samples from wild-type and mutant Anabaena strains grown under various conditions. Using advanced techniques such as gas chromatography (GC-MS), nuclear magnetic resonance (NMR), and matrix-assisted laser desorption ionization (MALDI) MS, the project will identify monomer composition, molecular weight, and branching patterns of EPS. Linkage analysis will provide detailed insights into glycosidic bond configurations, critical for predicting material properties. Additionally, size-exclusion chromatography will be employed to determine molecular weight distribution and its correlation with mechanical properties, such as viscosity and fiber strength. Ultimately, this research aims to define structure-property relationships within EPS, providing a foundation for engineering polysaccharides with tailored mechanical characteristics for specific biomaterial applications.	Biotechnology	Experimental	Biotechnology / Life Sciences / Chemistry
TAP-5 (SD)	sonali.das@iitb.ac.in	Sonali Das	Development of photothermal catalysts for sustainable conversion of carbon dioxide conversion	Converting CO2 into synthetic fuels and chemicals using sunlight holds tremendous prospects for establishing a sustainable carbon-neutral economy. This project aims at developing tailormade photothermal catalysts with precise nanostructures (such as hierarchical core-shell/ yolk-shell structures) that can synergistically harvest light and heat to convert CO2 to fuels. The work will involve development of new nanomaterials (such as MOFs, core-shell catalysts), advanced material characterization, and catalyst testing studies, and reactor design. (https://sites.google.com/view/das-lab/research?authuser=0)	Catalysis & Reaction Engineering	Experimental	Chemical Engg/ Chemistry
TAP-6 (MT)	mahesh@che.iitb.ac.in	Mahesh Tirumkudulu	Building the next generation flow cytometer	A flow cytometer uses light scattering and fluorescent technique to measure size of particles and to detect presence of fluorescently tagged particles. Flow cytometers are used extensively in cancer detection, virology and infectious diseases. The goal of the project is to build a compact flow cytometer and will require concepts from fluid mechanics, colloids science and electronics. [1]	Biomedical devices, Fluid mechanics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical engineering, biomedical engineering, mechanical engineering, Physics

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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/):	Type of the project (TA, TAP or FA)
Only those candidates who have external fellowsip/s like CSIR/DBT JRF can opt for the following topis [FA-1 to FA-6]							
FA-1 (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
FA-2 (AtM)	amalani@iitb.ac.in	Ateeque Malani	Design of Porous Materials for Gas Storage and Separation	Hydrogen and methane storage is a critical challenge for realizing their potential as a clean energy carrier, especially in mobile and portable applications. Carbon-based porous materials such as activated carbons, graphene derivatives, and metal-organic frameworks (MOFs) have shown promise in their storage due to their high surface area, lightweight nature, and chemical stability. By utilizing molecular simulations along with organic synthesis, our group seek to optimize the structural and functional properties of these materials to enhance their gas adsorption capabilities for both storage and separation purpose.	Gas adsorption, porous materials, simulation, organic synthesis	Both: Theoretical (Computational or Modelling) + Experimental	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
FA-3 (AtM)	amalani@iitb.ac.in	Ateeque Malani	Design and Analysis of Clay-swelling Inhibitors	The petroleum industry is significantly challenged by clay swelling in subterranean formations, which occurs when hydrophilic clays absorb water, expanding in size and reducing the permeability of oil-bearing reservoirs. This phenomenon results in decreased oil recovery efficiency, increased production costs, and the potential for severe operational disruptions. Inhibiting clay swelling is therefore critical to improving oil extraction, particularly in shale and other clay-rich formations. Our aim is to use molecular simulations to rationally design inhibitors by analyzing structure-property relationships.	Clay-swelling, geoscience, interfacial systems	Theoretical / Computational / Modelling	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
FA-4 (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. 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	Physics, Physical Chemistry, Engineerign
FA-5 (SS)	saini@che.iitb.ac.in	Supreet Saini	Protein-protein interaction map of a cell.	Understanding how various components of a cell come together to interact, and result in a functioning unit called cell is a fundamental challenge of biology. In recent years, several high throughput experiments with bacteria and yeast have reported how proteins interact. In this project, we will study the logic of protein-protein interaction maps in yeast, and how these interactions can be used to design therapeutic interventions. [References: https://pmc.ncbi.nlm.nih.gov/articles/PMC2746753/ and https://www.science.org/doi/10.1126/science.278.5340.1064]	Computational Biology.	Theoretical / Computational / Modelling	Any background with quantitative training. Strong interest in learning biology and evolution.
FA-6 (JA)	adhikari@iitb.ac.in	Jhumpa Adhikari	Molecular Simulation Study Of Phase Change Materials for Thermal Energy Storage	https://sites.google.com/view/jhumpaadhikariiitb/research	Molecular Simulation	Theoretical / Computational / Modelling	Interest in coding
FA-7 (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-8 (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	Experimental	

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FA-9 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Chemical sensor development for water contaminants and technology for their removal	Continuous monitoring of water quality parameters, like total dissolved solids, heavy metals, inorganic ions, organic pollutants etc.is an important measurement, to ascertain quality and use of a water body. This is critical for both a flowing water-stream (river, canal) or a stagnant water-pool, like a lake. To that end, in this project, one has to work on a coated nanoparticle mediated, optical-spectra based sensor (developed by us)and also dye-based chemical reagants, which have been tested with both synthetic and field-water samples, for various species, like arsenic, fluoride, chromium, iron etc. The aim is to further develop the nanoparticle sensor solution/coating/reagant ratio optimization and study the material and interfacial properties of the sensor with contaminants in water, so as to further advance our current functional sensor platform with multiplexing abilities, suitable for field testing. Also, the work will entail miniaturization and coupling of water flow (for water sampling), mechanical autosampler, sensor-reagant and water-sample mixing devices and flow-cells to complete the device automation, as part of ongoing work in our laboratory. The next step will be to also develop methods to remove these measured contaminants, which we have achieved for arsenic, by using a nanoparticle coated polymeric fibre. Thus, this project will involve both sensing and removal of contaminants from water, with the final aim of providing clean, drinking water. Part of this work has been in collaboration with Electrical Engg. Dept., IITB and Industry partner from India and Japan. This will enable a broad understanding of different fields of engineering, during this research, in addition to one's own focus area of nanomaterials, sensing and water treatment. The project has been funded by DST and other agencies. Most of the work will be experimental, with some scope of modeling, depending on student's interest.	Water treatment	Experimental	Environmental, Chemistry, Materials, Chemical, Electrical, Mechanical
FA-10 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Development of polymeric implant for nanoparticle mediated drug delivery in pancreatic cancer	Pancreatic cancer is one of the cancers having the lowest 5-year survival rate, because of its late diagnosis and availability of only a couple of known drugs with very moderate increase in patient's survival. Based on our earlier work, we have shown that, nanoparticle mediated delivery of existing drugs can enhance the cytotoxicity in cancer cells. Accordingly, we have developed subcutaneous and orthotopic in-vivo experiments in mouse, in collaboration with Advanced Cancer Teaching Research and Education Centre (ACTREC), Navi Mumbai. The aim of this project will be to further increase the efficacy of this process, by making 3D printed, polymer-based implants in order to mimic the interaction of nanoparticles with cancer cells in a controlled microfluidic environment. The resulting insight will elucidate the optimization of the nanoparticle-based drug delivery system. We have already developed and further improving a film- and a gel-based implants. Some background or experimental exposure in any of the following is better: polymeric materials or nanomaterials or microfluidics or drug delivery. Chemical Engineering principles like transport phenomena, reaction engineering and life-sciences oriented skills in cell cultures, drug loading, release, cell dynamics will be useful. The project is funded by WRCB, IIT Bombay and it will be a work leading to learning and expertise in interdisciplinary research areas in chemical engineering, material science and biotechnology. The work will be in a group of students involving others already working in related parts of this project and clinical doctors, for final feedback on product developed. The work will be mostly experimental, with some scope of modeling based on student's interest.	Polymeric implant	Experimental	Biosciences, Chemistry, Materials, Chemical Engg., Mechanical

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FA-11 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Engineering nanoparticle size and shape: Multiscale modeling, simulation and applications	Nanoparticles show new and interesting properties different from bulk materials due to their extremely small size (diameter), large specific surface area and spatial anisotropy. It is thus critical to understand the variables that control its synthesis, leading to a desired application. Control of mean nanoparticle size, particle size distribution and specially, anisotropic particle shapes is the first step in many of these applications, involving enhanced adsorption and reaction rates. To gain further insight into the mechanism of formation of nanoparticles, we have already developed models on how individual nanoparticles form by processes like multiphase mass transfer, reaction, nucleation, Brownian collision, surface growth, coagulation and Ostwald ripening, followed by interparticle forces and differential growth rates along different crystal facets, leading to anisotropic particles. With the above mechanism in place, in this project, one has to build on our existing mesoscale mathematical models (population balance equations) and computer simulation (kinetic Monte Carlo) codes to apply for nanoparticle formation and growth in microemulsions, macroemulsions and bulk solvents. In conjunction, one can also carry out experiments, if required, involving other complex nanostructures, like core-shell or oval and flower-shaped nanoparticles, besides cylindrical nanorods. Copper/silver/gold as metallic and iron oxide/zinc oxide/silica as metal oxide nanoparticles will be considered as typical model systems, since we are already using them, for different applications, like, chemical sensing, water purification devices, catalysis and drug delivery. Thus, the student can only perform multiscale computational research (using population balance equation or kinetic Monte Carlo simulation) or do a combination of experiments and modeling. Depending on the student's interest, there would be further scope to use the model and simulation predictions with available or new experimental data, for improving these exciting applications of nanotechnology. Finally, exploring whether anisotropic particles can display enhanced reactivity, is of paramount importance, as it will open up a new paradigm in reaction engineering. This will lead to enhancement in rates of existing or new chemical reactions, utilizing such particles as catalysts. It can be a potential new paradigm in reaction engineering.	Nanoparticles	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engg., Mechanical, Physics, Materials
FA-12 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Chemical sensor development for water contaminants and technology for their removal	Continuous monitoring of water quality parameters, like total dissolved solids, heavy metals, inorganic ions, organic pollutants etc.is an important measurement, to ascertain quality and use of a water body. This is critical for both a flowing water-stream (river, canal) or a stagnant water-pool, like a lake. To that end, in this project, one has to work on a coated nanoparticle mediated, optical-spectra based sensor (developed by us)and also dye-based chemical reagants, which have been tested with both synthetic and field-water samples, for various species, like arsenic, fluoride, chromium, iron etc. The aim is to further develop the nanoparticle sensor solution/coating/reagant ratio optimization and study the material and interfacial properties of the sensor with contaminants in water, so as to further advance our current functional sensor platform with multiplexing abilities, suitable for field testing. Also, the work will entail miniaturization and coupling of water flow (for water sampling), mechanical autosampler, sensor-reagant and water-sample mixing devices and flow-cells to complete the device automation, as part of ongoing work in our laboratory. The next step will be to also develop methods to remove these measured contaminants, which we have achieved for arsenic, by using a nanoparticle coated polymeric fibre. Thus, this project will involve both sensing and removal of contaminants from water, with the final aim of providing clean, drinking water. Part of this work has been in collaboration with Electrical Engg. Dept., IITB and Industry partner from India and Japan. This will enable a broad understanding of different fields of engineering, during this research, in addition to one's own focus area of nanomaterials, sensing and water treatment. The project has been funded by DST and other agencies. Most of the work will be experimental, with some scope of modeling, depending on student's interest.	Water Treatment	Experimental	Chemical Engg., Environmental, Mechanical, Electrical, Materials, Chemistry
FA-13 (GAV)	ganeshav@iitb.ac.in	Ganesh Viswanathan	Countering tumor growth by enhancing cell death	Tumor cells evade cell-death. Tilting the cancer cell fate from proliferation to cell-death is an emerging therapeutic paradigm. The goal of this project is to unravel the cell signalling governing cell-death induced by the cytokine TNFa, present in large quantities in the tumor microenvironment. To achieve this, the project will involve construction of a literature curated reaction network, development of discrete kinetic model, and performing systematic simulations. Model will be constrained with in-house generated experimental measurements. Perturbation analysis will be used to identify approaches that may enable the tilting of cellular response from proliferation to cell-death. For more details, see https://sites.google.com/iitb.ac.in/ganesh/publications	Systems and Network Biology	Theoretical / Computational / Modelling	B.Tech/M.Tech in Chemical Engg/Biotechnology; M.Sc Physics/Math
FA-14 (JS)	jyotiseth@iitb.ac.in	Jyoti Seth	Engineering Crystallization: Shape Control Using Polymers and Colloidal Particles	Controlling crystal shape during crystallization is key to tailoring material properties like dissolution rate, flowability, and strength. By using growth-modifying agents such as polymers or colloidal particles, it's possible to influence crystal morphology, optimizing performance across applications like pharmaceuticals, pigments, and energy materials. This study aims to unlock new possibilities for material design by studying the influence of larger molecules like polymers and polymeric surfactants on crystal growth.	Crystallisation	Both: Theoretical (Computational or Modelling) + Experimental	Chemistry / Physics

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FA-15 (JS)	jyotiseth@iitb.ac.in	Jyoti Seth	Simulating the Rheology of Aspherical Particle Networks	We are developing advanced computational models to understand how the shape, size, and interactions of non-spherical particles influence the flow and mechanical properties of concentrated suspensions, gels, and colloidal networks. The successful candidate will work with cutting-edge simulation techniques, including discrete element modeling (DEM) and computational fluid dynamics (CFD), to explore the fundamental mechanisms governing particle rearrangement, yielding behavior, and viscoelastic properties. We will also explore integration of AI/ML into the rheology simulations. This research will provide critical insights for a range of applications, from industrial formulations to bio-materials, where precise control over rheology is essential.	DEM Simulations	Theoretical / Computational / Modelling	Chemical Engg / Chemistry / Physics / Mechanical Engg
FA-16 (AmS)	amol.subhedar@iitb.ac.in	Amol Subhedar	A lattice Boltzmann diffuse interface model for two-phase flow with moving solid boundaries	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. The project will involve building and testing a mathematical model with a C++ code. Example of application can be found in this paper:https://drive.google.com/file/d/1ncWfxN53uVnzDNVduOoKp6vUk_iBf5lo/view?usp=sharing	CFD, mathematical modeling	Theoretical / Computational / Modelling	Any engineering stream
FA-17 (BKS)	bharat.k.suthar@gmail.com	Bharatkumar Suthar	Na-ion battery: exploring the capacity fade of anode	The development of a robust performance and capacity fade model for Na-ion battery (NIB) hard carbon anodes is critical to addressing key challenges in the commercialization and long-term viability of this emerging energy storage technology. Hard carbon is considered a promising anode material due to its high theoretical capacity and affordability, but it suffers from various challenges, including irreversible capacity loss, cycling instability, and side reactions. Understanding the mechanisms of these failures is essential for improving NIB efficiency, lifespan, and safety. A detailed model can capture the dynamic electrochemical processes, such as sodium ion intercalation, solid-electrolyte interphase (SEI) formation, and structural changes in the hard carbon material, providing insights into the dominant factors driving capacity fade. By developing such a model, researchers can predict performance under different operating conditions, optimize material design, and guide the development of next-generation Na-ion batteries with enhanced durability and cost-effectiveness.	Batteries	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engg/Physics/Mechanical, coding experiance desirable. courses: Transport phenomena, reaction engineering, heat transfer
FA-18 (SwB)	swaticb@che.iitb.ac.in	Swati Bhattacharya	Molecular Simulations of HIV-2 protein VpX	Our research group is primarily engaged in the investigation of protein dynamics and mechanisms with applications to intrinsic immunity and viral response, HIV therapeutics and enzymatic catalysis. The Ph.D project involves research into an HIV-protein called VpX that enables viruses such as HIV-2 to oppose the host cell defences. The project involves using molecular dynamics simulations to get a mechanistic understanding of the interaction between the mammalian protein SAMHD1 and the retroviral protein VpX which could pave the way for the development of a new generation of anti-HIV drugs. The student will learn state of the art molecular simulations techniques and a variety of data-mining techniques that will enable them to process the trajectories. We will also look at possible therapeutics that can counteract VpX. The project will train students in computational biology, as well as in Machine Learning and data mining techniques that are widely used.	Biomolecular Simulations	Theoretical / Computational / Modelling	We welcome students from Chemical Engg/Physics/Chemistry/Biotech backgrounds. We are looking for students who are interested in computational work.An enthusiasm for modelling and simulations is required and an interest in learning to code is required.
FA-19 (SwB)	swaticb@che.iitb.ac.in	Swati Bhattacharya	Molecular Dynamics Study of Intrinsically Disordered Proteins: Mechanisms of disease and therapeutics	Proteins are essential for biological functions. While normally, we think of proteins as having a rigid structures, some are more dynamic than others. Intrinsically disordered proteins (IDPs) are those without a fixed, rigid structure, and can change their conformation a lot. This is, in fact, necessary for their function. IDPs are important in many functions such as cellular signalling and have also been implicated in many diseases, from Alzheimer's, type 2 diabetes mellitus to Parkinsons. Our lab has developed a set of tools to model the kinetics of such proteins. In this project, we will apply the set of tools to some IDPs to understand their dynamics. The method will give a fine-grained view of the kinetics of the IDP. Our focus is on amyloid oligomers implicated in various diseases. We will also study potential drugs that can interact with these molecules.This is a computational project with an emphasis on method development.The student will also be trained in performing molecular dynamics simulations and machine learning techniques.	Biomolecular Simulations	Theoretical / Computational / Modelling	We are looking for candidates who are keen on modelling and simulations and are interested in learning to code. Students of Chem. Engg/Chemistry/Physics/Biotech-BioSciences background with an interest in computational work are welcome to apply. Experience in coding in any language is welcome.
FA-20 (HN)	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers (TA / FA)	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.	Biopolymer Physics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical (or Mech, Materials, Aerospace) Engg, Physics, Physical Chemistry
FA-21 (HN)	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	Theoretical / Computational / Modelling	Chemical (or Mech, Materials, Aerospace) Engg, Physics, Physical Chemistry

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List of TA topics that will be available for PhD students selected under TA cetegory in Dec 2024 admission round.

All candidates who have applied under TA/RA/FA category are eligible to opt for TA choice.

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TA-A	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-B	amalani@iitb.ac.in	Ateeque Malani	Design of Porous Materials for Gas Storage and Separation	Hydrogen and methane storage is a critical challenge for realizing their potential as a clean energy carrier, especially in mobile and portable applications. Carbon-based porous materials such as activated carbons, graphene derivatives, and metal-organic frameworks (MOFs) have shown promise in their storage due to their high surface area, lightweight nature, and chemical stability. By utilizing molecular simulations along with organic synthesis, our group seek to optimize the structural and functional properties of these materials to enhance their gas adsorption capabilities for both storage and separation purpose.	Gas adsorption, porous materials, simulation, organic synthesis	Both: Theoretical (Computational or Modelling) + Experimental	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
TA-C	amalani@iitb.ac.in	Ateeque Malani	Design and Analysis of Clay-swelling Inhibitors	The petroleum industry is significantly challenged by clay swelling in subterranean formations, which occurs when hydrophilic clays absorb water, expanding in size and reducing the permeability of oil-bearing reservoirs. This phenomenon results in decreased oil recovery efficiency, increased production costs, and the potential for severe operational disruptions. Inhibiting clay swelling is therefore critical to improving oil extraction, particularly in shale and other clay-rich formations. Our aim is to use molecular simulations to rationally design inhibitors by analyzing structure-property relationships.	Clay-swelling, geoscience, interfacial systems	Theoretical / Computational / Modelling	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
TA-D	saini@che.iitb.ac.in	Supreet Saini	Protein-protein interaction map of a cell.	Understanding how various components of a cell come together to interact, and result in a functioning unit called cell is a fundamental challenge of biology. In recent years, several high throughput experiments with bacteria and yeast have reported how proteins interact. In this project, we will study the logic of protein-protein interaction maps in yeast, and how these interactions can be used to design therapeutic interventions. [References: https://pmc.ncbi.nlm.nih.gov/articles/PMC2746753/ and https://www.science.org/doi/10.1126/science.278.5340.1064]	Computational Biology.	Theoretical / Computational / Modelling	Any background with quantitative training. Strong interest in learning biology and evolution.
TA-E	wangikar@iitb.ac.in	Pramod Wangikar	Metabolic Pathway Optimization for Enhanced Exopolysaccharide (EPS) Production in Cyanobacteria: A Systems Biology Approach	This research seeks to uncover and optimize the metabolic pathways responsible for high-rate exopolysaccharide (EPS) production in Anabaena 33047, a cyanobacterial strain with potential applications in sustainable biomanufacturing. By employing a systems biology framework, we will analyze gene expression, metabolic flux distributions, and regulatory networks integral to EPS biosynthesis. A combination of targeted and untargeted metabolomics, using LC-MS, will be used to map intracellular and extracellular metabolite concentrations, identifying pathway bottlenecks and congestion points. Furthermore, 13C isotope-assisted Metabolic Flux Analysis (INST-MFA) will trace carbon fluxes through essential pathways, including the Calvin cycle, glycolysis, and the TCA cycle, under varying growth and EPS-producing conditions. By integrating multi-omics data with the genome-scale model iAnC892, constrained using transcriptional and 13C-MFA data, we aim to simulate and redesign metabolic fluxes. In collaboration with Prof. Suvarn Kulkarni of Chemistry Department and Prof. Yinjie Tang and Prof. Himadri Pakrasi at Washington University in St. Louis, this project will identify novel targets for genetic modification to enhance EPS yield and tailor product structure for specific industrial uses. The outcomes will contribute foundational insights to cyanobacterial metabolic engineering for bioresource optimization.	Biotechnology	Both: Theoretical (Computational or Modelling) + Experimental	Biotechnology / Life Sciences
TA-F	adhikari@iitb.ac.in	Jhumpa Adhikari	Molecular Simulation Study Of Phase Change Materials for Thermal Energy Storage	https://sites.google.com/view/jhumpaadhikariiitb/research	Molecular Simulation	Theoretical / Computational / Modelling	Interest in coding
TA-G	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-H	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	Experimental	

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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.):
TA-I	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Chemical sensor development for water contaminants and technology for their removal	Continuous monitoring of water quality parameters, like total dissolved solids, heavy metals, inorganic ions, organic pollutants etc.is an important measurement, to ascertain quality and use of a water body. This is critical for both a flowing water-stream (river, canal) or a stagnant water-pool, like a lake. To that end, in this project, one has to work on a coated nanoparticle mediated, optical-spectra based sensor (developed by us)and also dye-based chemical reagants, which have been tested with both synthetic and field-water samples, for various species, like arsenic, fluoride, chromium, iron etc. The aim is to further develop the nanoparticle sensor solution/coating/reagant ratio optimization and study the material and interfacial properties of the sensor with contaminants in water, so as to further advance our current functional sensor platform with multiplexing abilities, suitable for field testing. Also, the work will entail miniaturization and coupling of water flow (for water sampling), mechanical autosampler, sensor-reagant and water-sample mixing devices and flow-cells to complete the device automation, as part of ongoing work in our laboratory. The next step will be to also develop methods to remove these measured contaminants, which we have achieved for arsenic, by using a nanoparticle coated polymeric fibre. Thus, this project will involve both sensing and removal of contaminants from water, with the final aim of providing clean, drinking water. Part of this work has been in collaboration with Electrical Engg. Dept., IITB and Industry partner from India and Japan. This will enable a broad understanding of different fields of engineering, during this research, in addition to one's own focus area of nanomaterials, sensing and water treatment. The project has been funded by DST and other agencies. Most of the work will be experimental, with some scope of modeling, depending on student's interest.	Water treatment	Experimental	Environmental, Chemistry, Materials, Chemical, Electrical, Mechanical
TA-J	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Development of polymeric implant for nanoparticle mediated drug delivery in pancreatic cancer	Pancreatic cancer is one of the cancers having the lowest 5-year survival rate, because of its late diagnosis and availability of only a couple of known drugs with very moderate increase in patient's survival. Based on our earlier work, we have shown that, nanoparticle mediated delivery of existing drugs can enhance the cytotoxicity in cancer cells. Accordingly, we have developed subcutaneous and orthotopic in-vivo experiments in mouse, in collaboration with Advanced Cancer Teaching Research and Education Centre (ACTREC), Navi Mumbai. The aim of this project will be to further increase the efficacy of this process, by making 3D printed, polymer-based implants in order to mimic the interaction of nanoparticles with cancer cells in a controlled microfluidic environment. The resulting insight will elucidate the optimization of the nanoparticle-based drug delivery system. We have already developed and further improving a film- and a gel-based implants. Some background or experimental exposure in any of the following is better: polymeric materials or nanomaterials or microfluidics or drug delivery. Chemical Engineering principles like transport phenomena, reaction engineering and life-sciences oriented skills in cell cultures, drug loading, release, cell dynamics will be useful. The project is funded by WRCB, IIT Bombay and it will be a work leading to learning and expertise in interdisciplinary research areas in chemical engineering, material science and biotechnology. The work will be in a group of students involving others already working in related parts of this project and clinical doctors, for final feedback on product developed. The work will be mostly experimental, with some scope of modeling based on student's interest.	Polymeric implant	Experimental	Biosciences, Chemistry, Materials, Chemical Engg., Mechanical

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TA-K	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Engineering nanoparticle size and shape: Multiscale modeling, simulation and applications	Nanoparticles show new and interesting properties different from bulk materials due to their extremely small size (diameter), large specific surface area and spatial anisotropy. It is thus critical to understand the variables that control its synthesis, leading to a desired application. Control of mean nanoparticle size, particle size distribution and specially, anisotropic particle shapes is the first step in many of these applications, involving enhanced adsorption and reaction rates. To gain further insight into the mechanism of formation of nanoparticles, we have already developed models on how individual nanoparticles form by processes like multiphase mass transfer, reaction, nucleation, Brownian collision, surface growth, coagulation and Ostwald ripening, followed by interparticle forces and differential growth rates along different crystal facets, leading to anisotropic particles. With the above mechanism in place, in this project, one has to build on our existing mesoscale mathematical models (population balance equations) and computer simulation (kinetic Monte Carlo) codes to apply for nanoparticle formation and growth in microemulsions, macroemulsions and bulk solvents. In conjunction, one can also carry out experiments, if required, involving other complex nanostructures, like core-shell or oval and flower-shaped nanoparticles, besides cylindrical nanorods. Copper/silver/gold as metallic and iron oxide/zinc oxide/silica as metal oxide nanoparticles will be considered as typical model systems, since we are already using them, for different applications, like, chemical sensing, water purification devices, catalysis and drug delivery. Thus, the student can only perform multiscale computational research (using population balance equation or kinetic Monte Carlo simulation) or do a combination of experiments and modeling. Depending on the student's interest, there would be further scope to use the model and simulation predictions with available or new experimental data, for improving these exciting applications of nanotechnology. Finally, exploring whether anisotropic particles can display enhanced reactivity, is of paramount importance, as it will open up a new paradigm in reaction engineering. This will lead to enhancement in rates of existing or new chemical reactions, utilizing such particles as catalysts. It can be a potential new paradigm in reaction engineering.	Nanoparticles	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engg., Mechanical, Physics, Materials
TA-L	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Chemical sensor development for water contaminants and technology for their removal	Continuous monitoring of water quality parameters, like total dissolved solids, heavy metals, inorganic ions, organic pollutants etc.is an important measurement, to ascertain quality and use of a water body. This is critical for both a flowing water-stream (river, canal) or a stagnant water-pool, like a lake. To that end, in this project, one has to work on a coated nanoparticle mediated, optical-spectra based sensor (developed by us)and also dye-based chemical reagants, which have been tested with both synthetic and field-water samples, for various species, like arsenic, fluoride, chromium, iron etc. The aim is to further develop the nanoparticle sensor solution/coating/reagant ratio optimization and study the material and interfacial properties of the sensor with contaminants in water, so as to further advance our current functional sensor platform with multiplexing abilities, suitable for field testing. Also, the work will entail miniaturization and coupling of water flow (for water sampling), mechanical autosampler, sensor-reagant and water-sample mixing devices and flow-cells to complete the device automation, as part of ongoing work in our laboratory. The next step will be to also develop methods to remove these measured contaminants, which we have achieved for arsenic, by using a nanoparticle coated polymeric fibre. Thus, this project will involve both sensing and removal of contaminants from water, with the final aim of providing clean, drinking water. Part of this work has been in collaboration with Electrical Engg. Dept., IITB and Industry partner from India and Japan. This will enable a broad understanding of different fields of engineering, during this research, in addition to one's own focus area of nanomaterials, sensing and water treatment. The project has been funded by DST and other agencies. Most of the work will be experimental, with some scope of modeling, depending on student's interest.	Water Treatment	Experimental	Chemical Engg., Environmental, Mechanical, Electrical, Materials, Chemistry
TA-M	ganeshav@iitb.ac.in	Ganesh Viswanathan	Countering tumor growth by enhancing cell death	Tumor cells evade cell-death. Tilting the cancer cell fate from proliferation to cell-death is an emerging therapeutic paradigm. The goal of this project is to unravel the cell signalling governing cell-death induced by the cytokine TNFa, present in large quantities in the tumor microenvironment. To achieve this, the project will involve construction of a literature curated reaction network, development of discrete kinetic model, and performing systematic simulations. Model will be constrained with in-house generated experimental measurements. Perturbation analysis will be used to identify approaches that may enable the tilting of cellular response from proliferation to cell-death. For more details, see https://sites.google.com/iitb.ac.in/ganesh/publications	Systems and Network biology	Theoretical / Computational / Modelling	B.Tech/M.Tech in Chemical Engg/Biotechnology/Physics.
TA-N	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 Flow Modelling (CFD)	Theoretical / Computational / Modelling	Chemical Engineering OR Mechanical Engineering

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TA-O	jyotiseth@iitb.ac.in	Jyoti Seth	Engineering Crystallization: Shape Control Using Polymers and Colloidal Particles	Controlling crystal shape during crystallization is key to tailoring material properties like dissolution rate, flowability, and strength. By using growth-modifying agents such as polymers or colloidal particles, it's possible to influence crystal morphology, optimizing performance across applications like pharmaceuticals, pigments, and energy materials. This study aims to unlock new possibilities for material design by studying the influence of larger molecules like polymers and polymeric surfactants on crystal growth.	Crystallisation	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering or Chemistry or Physics
TA-P	jyotiseth@iitb.ac.in	Jyoti Seth	Simulating the Rheology of Aspherical Particle Networks	We are developing advanced computational models to understand how the shape, size, and interactions of non-spherical particles influence the flow and mechanical properties of concentrated suspensions, gels, and colloidal networks. The successful candidate will work with cutting-edge simulation techniques, including discrete element modeling (DEM) and computational fluid dynamics (CFD), to explore the fundamental mechanisms governing particle rearrangement, yielding behavior, and viscoelastic properties. We will also explore integration of AI/ML into the rheology simulations. This research will provide critical insights for a range of applications, from industrial formulations to bio-materials, where precise control over rheology is essential.	DEM Simulations	Theoretical / Computational / Modelling	Chemical Engg / Chemistry / Physics / Mechanical Engg
TA-Q	amol.subhedar@iitb.ac.in	Amol Subhedar	A lattice Boltzmann diffuse interface model for two-phase flow with moving solid boundaries	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. The project will involve building and testing a mathematical model with a C++ code. Example of application can be found in this paper:https: //drive.google.com/file/d/1ncWfxN53uVnzDNVduOoKp6vUk_iBf5lo/view?usp=sharing	CFD, mathematical modeling	Theoretical / Computational / Modelling	Any engineering stream
TA-R	bharat.k.suthar@gmail.com	Bharatkumar Suthar	Na-ion battery: exploring the capacity fade of anode	The development of a robust performance and capacity fade model for Na-ion battery (NIB) hard carbon anodes is critical to addressing key challenges in the commercialization and long-term viability of this emerging energy storage technology. Hard carbon is considered a promising anode material due to its high theoretical capacity and affordability, but it suffers from various challenges, including irreversible capacity loss, cycling instability, and side reactions. Understanding the mechanisms of these failures is essential for improving NIB efficiency, lifespan, and safety. A detailed model can capture the dynamic electrochemical processes, such as sodium ion intercalation, solid-electrolyte interphase (SEI) formation, and structural changes in the hard carbon material, providing insights into the dominant factors driving capacity fade. By developing such a model, researchers can predict performance under different operating conditions, optimize material design, and guide the development of next-generation Na-ion batteries with enhanced durability and cost-effectiveness.	Batteries	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engg/Physics/Mechanical, coding experiance desirable. courses: Transport phenomena, reaction engineering, heat transfer
TA-S	swaticb@che.iitb.ac.in	Swati Bhattacharya	Molecular Simulations of HIV-2 protein VpX	Our research group is primarily engaged in the investigation of protein dynamics and mechanisms with applications to intrinsic immunity and viral response, HIV therapeutics and enzymatic catalysis. The Ph.D project involves research into an HIV-protein called VpX that enables viruses such as HIV-2 to oppose the host cell defences. The project involves using molecular dynamics simulations to get a mechanistic understanding of the interaction between the mammalian protein SAMHD1 and the retroviral protein VpX which could pave the way for the development of a new generation of anti-HIV drugs. The student will learn state of the art molecular simulations techniques and a variety of data-mining techniques that will enable them to process the trajectories. We will also look at possible therapeutics that can counteract VpX. The project will train students in computational biology, as well as in Machine Learning and data mining techniques that are widely used.	Biomolecular Simulations	Theoretical / Computational / Modelling	We welcome students from Chemical Engg/Physics/Chemistry/Biotech backgrounds. We are looking for students who are interested in computational work.An enthusiasm for modelling and simulations is required and an interest in learning to code is required.
TA-T	swaticb@che.iitb.ac.in	Swati Bhattacharya	Molecular Dynamics Study of Intrinsically Disordered Proteins: Mechanisms of disease and therapeutics	Proteins are essential for biological functions. While normally, we think of proteins as having a rigid structures, some are more dynamic than others. Intrinsically disordered proteins (IDPs) are those without a fixed, rigid structure, and can change their conformation a lot. This is, in fact, necessary for their function. IDPs are important in many functions such as cellular signalling and have also been implicated in many diseases, from Alzheimer's, type 2 diabetes mellitus to Parkinsons. Our lab has developed a set of tools to model the kinetics of such proteins. In this project, we will apply the set of tools to some IDPs to understand their dynamics. The method will give a fine-grained view of the kinetics of the IDP. Our focus is on amyloid oligomers implicated in various diseases. We will also study potential drugs that can interact with these molecules.This is a computational project with an emphasis on method development.The student will also be trained in performing molecular dynamics simulations and machine learning techniques.	Biomolecular Simulations	Theoretical / Computational / Modelling	We are looking for candidates who are keen on modelling and simulations and are interested in learning to code. Students of Chem. Engg/Chemistry/Physics/Biotech-BioSciences background with an interest in computational work are welcome to apply. Experience in coding in any language is welcome.
TA-U	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers (TA / FA)	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.	Biopolymer Physics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical (or Mech, Materials, Aerospace) Engg, Physics, Physical Chemistry
TA-V	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	Theoretical / Computational / Modelling	Chemical (or Mech, Materials, Aerospace) Engg, Physics, Physical Chemistry