Department of Chemical Engineering, IIT Bombay.
List of TAP, FA, and TA Ph.D Topics for Autumn 2024-2025 (May 2025)
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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 (SV)	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay	Designing Green Hydrogen Electrocatalysts with Constant Potential First Principles Calculations and Machine Learning	Green hydrogen is one of the most promising clean energy sources of the future. Unlike current hydrogen production methods that rely on fossil fuels, hydrogen can be produced sustainably through electrochemical water splitting. For this process to be practical on an industrial scale, it must work efficiently under alkaline conditions, which are safer and more compatible with a wider range of materials than acidic environments. However, two major challenges stand in the way. First, we lack affordable, stable, and efficient catalysts that can drive the reaction. Second, we don't fully understand how the electrode–electrolyte interface (the region where water molecules, ions, and electric fields interact with the catalyst surface) affects the reaction mechanism. The Theoretical Electrocatalysis Group focuses on tackling both challenges using powerful quantum mechanical simulations. We apply density functional theory (DFT) to model how atoms and electrons behave during the hydrogen evolution reaction. What sets us apart is that we are currently the only group with the capability to perform truly constant potential DFT simulations without any implicit electrolyte treatment. This method allows us to study electrochemical reactions in a realistic environment, without introducing the common artifacts that affect other simulation methods. What you will do in the project: (1) Use DFT simulations to study how water molecules split and form hydrogen on different catalyst surfaces (2) Explore how nearby ions and the electric double layer affect reaction pathways and energy barriers (3) Use machine learning to accelerate these simulations and search for patterns in catalytic activity (3) Investigate new materials and develop design principles for next-generation hydrogen evolution catalysts Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group https://www.che.iitb.ac.in/web/faculty/sv	machine learning for science and engineering	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering or Chemistry and Physics who are curious about clean energy, catalysis, and computational modeling. You don't need prior experience in DFT or machine learning, just a willingness to learn.
	TAP-2 (NR)	nagappan@iitb.ac.in	Nagappan Ramaswamy	Electrocatalysts for Hydrogen Generation in Acidic Water Electrolyzers	1) Synthesize and develop iridium based electrocatalysts for water oxidation reaction in proton exchange membrane water electrolyzers 2) Evaluate the electrochemical activity and performance of iridium based electrocatalysts 3) Understand their degradation mechanisms under steady-state and dynamic operating conditions 4) Develop mechanistic understanding of the electrocatalyst using in situ spectroscopic measurements.	Green hydrogen generation	Experimental	Chemical engineering, Chemistry, Electrochemistry, Nanotechnology
	TAP-3 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Utilizing Polymer Physics to understand the effect of loop formation in chromatin dynamics	Loops often form in long biological molecules like DNA and play an important role in how these molecules are shaped and how they move. In particular, loops are crucial in understanding the structure and behavior of chromatin — the complex of DNA and proteins inside our cells. In this project, we will use ideas from **polymer physics* *to understand how loop formation affects the structure and motion of biopolymers. We'll also look at how the movement of a few points on a chromatin (as seen in experiments) can help us figure out whether a loop exists, and if so, where it starts and ends. To do this, we'll use statistical methods such as Bayesian inference. Overall, this project will demonstrate how physics can help us make predictions about the structure of chromatin using dynamic data. For more details of our work please visit:https://sites.google.com/view/sayantand2/	(Bio)Polymer Physics	Theoretical / Computational / Modelling	1. Training in Engineering/Physics/Physical Chemistry 2. Strong Quantitative/Computational Background 3. No biology background required
	TAP-4 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Computational Tissue Engineering for smart 3D bio-printing	In living tissues, cells don't just sit still — they move, stick to each other, multiply, and respond to their surroundings. These actions are what allow cells to organize themselves into complex tissues and organs. In this project, we aim to build a **biophysical simulation software** that mimics how cells behave and interact over time. We'll use particle-based models (similar to **Molecular Dynamics**) to model how cells move and organize themselves starting from a given structure. We Plan to validate our prediction using 3D bioprinting in collaboration with Dr, Tapomoy Bhattacharjee at NCBS. For more details about our work visit: https://sites.google.com/view/sayantand2/	Biophysics, Cell Mechanics	Theoretical / Computational / Modelling	1. Training in Engineering/Physics/Physical Chemistry 2. Strong Quantitative/Computational Background 3. No biology background required
	TAP-5 (RaD)	dasgupta.ratul@iitb.ac.in	Ratul Dasgupta	Direct numerical simulations of turbulent flow of charged suspensions	This project is under the supervision of Prof. Ravichandran (Climate Studies) and will be co-supervised by me. The student will need to carry out extensive DNS guided by theory. Applications in cloud microphysics.	Fluid Mechanics	Theoretical / Computational / Modelling	Chemical / Mechanical / Aerospace / Physics
	TAP-6 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Complete water quality monitoring system for physicochemical parameters and pollutants, by automated, real-time, remote measurement of waterbodies	We have already developed in our lab. an autonomous device for real-time, water quality monitoring by both physical and chemical sensors (some of the sensors being developed by us), withyears of work by a multidisciplinary team. We will further combine both types of sensors in a single device, via basic research on these sensors for metal detection. Funded under the theme 'Environment & Sustainability' of GESH, IIT Bombay, further objectives of this project are: (i)monitoring multiple, individual water-bodies and then later measuring connected water streams and water bodies. This will further allow, (ii)possible prediction of short-term behaviour of physical and chemical parameters of isolated water bodies, (iii)facilitation of tracking the origin of a pollutant downstream of a water-stream, possibly by the method of source apportionment of input streams feeding into it, (iv)identification of clean, moderately polluted and highly polluted zones in a wider region, as a possible prelude to a water-pollution map. Thus one has to have either some background or interest in chemical, environmental, materials engg. for basic research or have liking of designing and fabricating of electromechanical devices, to fit into our current team and carry out PhD research. [1]	Water sensors for environmental monitoring	Experimental	Chemical Engg., Environmental Engg., Materials Engg., Mechanical Engg., Electrical Engg

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	TAP-7 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Designing Shape and Patterns in Artificial Tissues Using Computational Models	In nature, complex living organisms begin as a single cell that divides and grows into tissues and organs. As this happens, chemical signals create patterns inside the tissues, which in turn affect how the tissue grows and changes shape. Inspired by how this works in real organisms, this project aims to build a **computational tool based on chemical engineering principles** that can help us design artificial tissues that grow and form specific patterns and shapes. Specifically, we plant to develop a PDE based computational tool integrating **transport phenomena, reaction kinetics, and solid mechanics**. Utilizing this tool, we aim to create "digital tissues" that mimic how real tissues grow and change. This approach could eventually help in designing artificial tissues or implants that naturally develop into desired shapes and functions. For More details about our work please visit: https://sites.google.com/view/sayantand2/team	Pattern formation, Biophysics	Theoretical / Computational / Modelling	1. Training in Engineering/Physics/Physical Chemistry 2. Strong Quantitative/Computational Background specifically numerical methods 3. No biology background required
	TAP-8 (SD)	sonali.das@iitb.ac.in	Sonali Das	Catalyst development for green hydrogen applications (liquid hydrogen carriers)	This project aims at the development of new catalysts and catalytic processes for the conversion of hydrogen into liquid hydrogen carriers and vice versa, which is an important step towards establishing a sustainable green hydrogen economy. The work would entail development of new catalyst materials, characterization, testing catalyst performance in reactors and detailed kinetic studies for green H2 applications.	Catalysis, Green Hydrogen, Sustainability	Experimental	
	TAP-9 (SMe)	sarika@che.iitb.ac.in	Sarika Mehra	Modelling the transmission of infectious diseases	Epidemiological models such as SIR are used to model the transmission of infectious diseases in the population. In this project, we will expand these models to incorporate the biology of both the host and the pathogen. We also plan to explore various modelling paradigms for understanding the transmission of disease in the population.	mathematical model	Theoretical / Computational / Modelling	Chemical Engineering/Computational Biology Knowledge of coding essential

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	Only those candidates who have external fellowsip/s like CSIR/DBT JRF can opt for the following topis [FA-1 to FA-46]							
	FA-1 (AS)	a.sarkar@iitb.ac.in	Arindam Sarkar	Investigations on electrochemical CO2 reduction to formate and other C1/C2 chemicals	This is an experimental research project centered on the electrochemical reduction of carbon dioxide (CO_2) into formate or other high-value chemical products (1,2). The work will explore the design, synthesis, and application of metal and alloy-based catalysts, with a particular emphasis on their integration into gas diffusion electrodes (GDEs). These electrodes will be tested and optimized within a novel electrochemical setup, primarily utilizing a two-electrode flow cell configuration, although a three-electrode system may also be employed for more detailed mechanistic studies. The experimental tasks will involve the synthesis of nanoparticles and catalytic materials, followed by comprehensive physico-chemical and electrochemical characterization. Techniques may include, but are not limited to, transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and cyclic voltammetry (CV). The products will be analyzed using HPLC/GC. Although prior experience in electrochemistry is not a prerequisite, the student is expected to develop a strong foundation in advanced electroanalytical techniques and physical characterization methods over the course of the project. This experience will be integral to understanding catalyst performance and reaction mechanisms in CO_2 electroreduction systems. The project is experimental in nature. (1) Al-Tamreh, S. A.; Ibrahim, M. H.; El-Naas, M. H.; Vaes, J.; Pant, D.; Benamor, A.; Amhamed, A. Electroreduction of Carbon Dioxide into Formate: A Comprehensive Review. ChemElectroChem 2021, 8 (17), 3207–3220. https://doi.org/10.1002/celc.202100438. (2) Giri, S. D.; Mahajani, S. M.; Suresh, A. K.; Sarkar, A. Electrochemical Reduction of CO2 on Activated Copper: Influence of Surface Area. Materials Research Bulletin 2020, 123, 110702. https://doi.org/10.1016/j.materresbull.2019.110702.	Electrochemistry	Experimental	
	FA-2 (AS)	a.sarkar@iitb.ac.in	Arindam Sarkar	Investigating the Underlying Unity of Chemical and Electrochemical Processes	It has been reasonably established that catalytic chemical oxidation and electrochemical oxidation are not fundamentally different or unrelated processes. Rather, they appear to be different manifestations of the same underlying electrochemical mechanism. In this context, the project aims to develop a more unified framework for comparing chemical and electrochemical oxidation pathways, building on the work conducted by previous students. The selected candidate will be expected to extend this research and rigorously investigate the equivalence between chemical and electrochemical oxidation mechanisms, particularly in non-aqueous systems. A key focus will be on understanding the role of dopants and poisons in modulating these pathways. At a later stage, the project may also involve the synthesis of nanoparticulate catalysts. While prior experience in electrochemistry is not mandatory, the student should possess a strong interest in analytical electrochemistry and detailed analysis of current–voltage behavior and reaction mechanisms. The project is experimental in nature with a small degree of modelling. (1) Chauhan, N. L.; Dameera, V.; Juvekar, V. A.; Mahajani, S. M.; Suresh, A. K.; Sarkar, A. Correlation of Chemical and Electrochemical Catalysis-Importance of Half Reactions: The Case of Catalytic Oxidation of Ferrous Sulfate by Molecular Oxygen. Journal of The Electrochemical Society 2018, 165 (5), H196–H204. (2) Chauhan, N. L.; Juvekar, V. A.; Sarkar, A. Oxidation of Ethylene Glycol: Unity of Chemical and Electrochemical Catalysis. Electrochemical Science Advances 2022, 2 (6), e2100092.	Electrochemistry	Experimental	
	FA-3 (AS)	a.sarkar@iitb.ac.in	Arindam Sarkar	Electrosynthesis of hydrogen peroxide	This project focuses on the design and development of advanced catalysts and electrochemical cell configurations to enable efficient, selective, and sustainable electrosynthesis of hydrogen peroxide (H_2O_2). Hydrogen peroxide is a valuable green oxidant with wide-ranging applications in environmental remediation, chemical manufacturing, and healthcare. However, traditional methods of H_2O_2 production, such as the anthraquinone process, are energy-intensive and centralized, posing environmental and economic limitations. The proposed research aims to address these challenges by investigating electrochemical pathways for in situ H_2O_2 generation, particularly via the two-electron oxygen reduction reaction ($2e^-$ ORR). Key goals include (a) Synthesizing and characterizing transition-metal-based or alloy catalysts with high selectivity toward the $2e^-$ ORR pathway. (b) fabricating tailored electrodes, including gas diffusion electrodes and porous structures, to support efficient mass transport and electron transfer. Electrochemical cells—ranging from H-type cells to flow cells—will be developed and optimized to enhance H_2O_2 productivity and scalability, and (c) Systematic testing of catalyst-electrode-cell systems under various operating conditions (e.g., electrolyte composition, pH, applied potential, temperature) to maximize Faradaic efficiency, H_2O_2 concentration, and long-term stability. The project is experimental in nature. (1) Shi, X.; Back, S.; Gill, T. M.; Siahrostami, S.; Zheng, X. Electrochemical Synthesis of H2O2 by Two-Electron Water Oxidation Reaction. Chem 2021, 7 (1), 38–63. https://doi.org/10.1016/j.chempr.2020.09.013. (2) Perry, S. C.; Pangotra, D.; Vieira, L.; Csepei, L.-I.; Sieber, V.; Wang, L.; Ponce de León, C.; Walsh, F. C. Electrochemical Synthesis of Hydrogen Peroxide from Water and Oxygen. Nat Rev Chem 2019, 3 (7), 442–458. https://doi.org/10.1038/s41570-019-0110-6.	Electrochemistry	Experimental	
	FA-4 (AtM)	amalani@IITB.ac.in	Ateeque Malani	Design and Synthesis of Porous Materials for natural gas storage	Natural gas (NG) has very low energy density compared to diesel and petrol, hence NG is often compressed or liquefied to increase it. The process of compression or liquefaction are often costly and has serious safety issues. An alternative is to adsorb NG in porous materials. The aim of this project is to use computational approach to design novel porous materials and synthesise them using experimental approach.	Natural Gas, Energy, Porous Materials	Both: Theoretical (Computational or Modelling) + Experimental	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
	FA-5 (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-6 (AtM)	amalani@IITB.ac.in	Ateeque Malani	Simulation studies of enhanced oil recovery	With increase in energy demand, the requirement of crude oil is expected to increase worldwide. The current oil production rates are significantly affected due to depletion of oil from existing reservoirs. Thus to increase production rates, enhanced oil recovery approach needs to be adopted. However, current approach is mostly heuristic and practise based. The aim of this project is use chemical engineering fundamentals to study enhance oil recovery process to design guidelines.	Energy, Oil recovery	Theoretical / Computational / Modelling	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
	FA-7 (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

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	FA-8 (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-9 (GAV)	ganeshav@iitb.ac.in	Ganesh Viswanathan	Kinetic modelling of cell-death	Cell-death process, which occurs ubiquitously under normal and healthy conditions, is disturbed in diseased tissues. Cell-death process can be viewed as an outcome of a network of biochemical reactions, activated by a certain stimulus. How does the network dynamically orchestrate the overall cell-death outcome? Can the network be re-wired to reverse the disturbances in the cell-death process? The goal of this project is to understand the cell-death process by developing a kinetic model of the underlying signalling network and validating with experimental measurements, available in-house. This inter-disciplinary project will involve simulating the model to generate big data and analysing the same using appropriate tools such as those from machine learning.	Systems biology	Theoretical/Computational	Chemical Engineering/Biotechnology/Bioengineering/Physics. Candidate must have completed linear algebra and basic biology courses.
	FA-10 (GAV)	ganeshav@iitb.ac.in	Ganesh Viswanathan	Long-term response of a tumour	Tumor necrosis factor alpha (TNFa), a pleiotropic cytokine is implicated in several pathological conditions such as cancer. Besides, TNFa is an important component of the cytokine storm observed in COVID19 patients causing strong lung-inflammation. TNFa is capable of making the triggered cells take different long-term phenotypic response such as pro-survival or apoptotic or necroptotic state. Why and how cells permit such multiple responses? Can the underlying signal transduction network consisting of biochemical reactions be modulated dynamically to enable phenotype switching? The objective of this inter-disciplinary project is to develop systems biology based models of the network to identify strategies for phenotype switching from pro-survival to apoptosis/necroptosis. The project will primarily involve modeling and simulations, and subsequently contrasting the model predictions with experimental data.	Systems biology	Theoretical/Computational	Chemical Engineering/Biotechnology/Bioengineering/Physics. Candidate must have completed linear algebra and basic biology courses.
	FA-11 (GK)	guruswamy@iitb.ac.in	Guruswamy Kumaraswamy	Sustainable bio-derived polymers: Structure-property relations	Bioderived polymers represent a possible solution to the problem of plastic pollution. However, to replace the dominant synthetic polymers such as polyethylene and polypropylene, these polymers will need to have suitable balance of properties. The properties of polymers are governed by their (often non-equilibrium) structure. This project will aim at developing suitable bioderived polymer substitutes (such as cellulosics, algal polysaccharides or polyhydroxyalkanoates) for specific circular applications. This is primarily experimental and will involve rheology, thermal analysis, scattering and solid property measurements. There is also a possibility of collaboration with industry partners.	Sustainable bioderived polymers	Experimental	No specific background
	FA-12 (GK)	guruswamy@iitb.ac.in	Guruswamy Kumaraswamy	Formation of micro and nanoplastics	The annual global production of synthetic plastics is of the order of 400 million tons. A majority of these materials are improperly disposed and undergo environmental degradation. This results in the formation of particulate pollutants, micro and nanoplastics. Understanding how plastics degrade to form such pollutants is an area of great contemporary importance. In this project, we will explore the fundamental principles that guide the degradation of plastics and how this results in the formation of micro and nanoplastics. This is primarily an experimental project, and will involve a wide swathe of characterization techniques, that are available in the institute. Interested students can refer to some recent papers from our group in this area (nature.com/articles/s41467-025-58233-3 and https://doi.org/10.1039/D5SM00074B)	Microplastics	Experimental	No specific background
	FA-13 (HN)	hnanavati@iitb.ac.in	Hemant Nanavati	Accurate Molecular Models for Real Polymers	We develop compact, closed form, but accurate molecular models as well as elasticity relationships for real polymers, incorporating structural aspects. The applications include synthetic (e.g., those used as matrix for solid propellant) as well as high performance Bio-sourced polymers.	Polymer Physics	Theoretical / Computational / Modelling	Chemical Engg/Chemistry/Physics/ Materials Science/Polymers/ Knowledge of coding
	FA-14 (HN)	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of 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.	Biopolymer Physics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engg/Chemistry/Physics/ Materials Science/Polymers/ Knowledge in coding
	FA-15 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth	Why Do Like-Charged Polymers Stick Together? Exploring Polyethylenimine in Acidic Water	Normally, materials with the same charge repel each other. But in some cases—like with the polymer polyethylenimine (PEI) in acidic water—they actually come together and form fascinating structures. This PhD project will use computer simulations (and maybe some expeirments) to figure out why this happens. You'll dive into the tiny world of molecules to see how acid levels, ions, and water molecules affect the way these polymers behave. The results could help improve things like gene delivery in medicine. If you're into soft matter, modeling, simulations, or nanoscale interactions—this is for you!	self assembly	Both: Theoretical (Computational or Modelling) + Experimental	Skills You'll Need or Develop: Molecular dynamics simulations (e.g., GROMACS, LAMMPS, or similar), Basic programming (Python or similar for data analysis and scripting), Understanding of thermodynamics and intermolecular forces, Data visualization and analysis, understanding of soft matter or nanomaterials No worries if you don't have all of these yet—this PhD is designed to help you build them
	FA-16 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth	Multiscale Modeling of Crystallization Dynamics	This PhD project aims to explore how crystals grow in solutions. The research will use computer simulations along with a few carefully designed experiments to study how crystals start to form, how fast they grow, and how certain chemicals—called additives—can help or slow down this process. By combining models that look at both small-scale (molecular) and larger-scale behaviors, the project will give a clearer picture of what controls crystal growth. These insights are important for improving processes in medicine, materials design, and electronics.	Crystallisation	Both: Theoretical (Computational or Modelling) + Experimental	The ideal candidate should have a background in chemistry, chemical engineering, physics, materials science, or a related field, and a strong interest in learning new techniques. During the PhD, the candidate will be trained in: Computer modeling and multiscale simulation methods Basic programming (e.g., Python, MATLAB) Experimental techniques related to crystallization Data analysis and scientific communication Strong problem-solving skills and curiosity about molecular processes are highly valued. No prior experience in simulations or crystallization is mandatory as requisite training will be provided as part of the project.

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	FA-17 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth	Modeling the Dynamics and Flow Behavior of Non-Newtonian Fluids	This PhD project will study how complex fluids behave when they flow and how certain additives—like polymers, nanoparticles, and surfactants—can change their flow properties. Using computer simulations and special programs, the research will look at how factors like temperature, pressure, and concentration affect fluid flow. The aim is to create a model that helps design better materials and additives for improving the performance of fluids in industries like oil, medicine, and materials science.	Fluid mechanics	Both: Theoretical (Computational or Modelling) + Experimental	The ideal candidate will have a background in chemical engineering, physical chemistry, materials science, or a closely related field. During the PhD, the candidate will gain expertise in: Fluid dynamics, Molecular dynamics simulations, utilizing platforms like GROMACS or LAMMPS Computational modeling of rheological properties Advanced data analysis, visualization techniques, and statistical modeling Fundamental principles of rheology and material behavior in complex fluids Scientific writing, communication, and presentation skills Prior experience with computational simulations or programming is advantageous but not required—full training will be provided throughout the PhD.
	FA-18 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth	Simulating the Elasticity of Soft Materials for Biomedical and Environmental Applications	This PhD project will explore how the size, shape, and connectivity of nanoparticles or microparticles influence the strength, flexibility, and performance of materials such as tissue engineering scaffolds, clays, hydrogels, and oleogels. By using advanced computer simulations, we will analyze how these particles interact to form networks, how their connectivity impacts material properties, and how the networks respond under stress. A few experiments may also be performed to validate and complement the simulation results. The aim is to develop a predictive tool that enables the design of materials with optimal strength, flexibility, and network connectivity. This research will be valuable for industries ranging from biomedical engineering (e.g., tissue scaffolds), pharmaceuticals (e.g., drug delivery systems), materials science (e.g., hydrogels and oleogels for various applications), and environmental engineering (e.g., clay-based filtration materials).	Colloids and Soft Matter	Both: Theoretical (Computational or Modelling) + Experimental	Degree in Chemical Engineering, Chemistry, Physics, Materials Science, or related field. Familiarity with material characterization (rheology, microscopy), material preparation (hydrogels, oleogels), and mechanical testing is beneficial Computational Skills: Knowledge of computational modeling (particle simulations), coding (Python, MATLAB), and simulation software (e.g., GROMACS, LAMMPS) is a plus; training will be provided. Note: The candidate need not have all the skills listed but will be trained during the course of the project.
	FA-19 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth	Energy-Efficient Methods for Clearing Wax Blockages in Crude Oil Pipelines Using Electric Fields	This PhD project will explore innovative methods to clear wax blockages in crude oil pipelines, building on previous research that demonstrates how electric fields can effectively break down wax networks, converting them into low-viscosity liquids that flow more easily. The research will investigate how electric fields can be applied to disrupt wax buildup, ensuring continuous oil flow. Additionally, the project will assess the design of devices to generate these electric fields, the impact of electric fields on wax, and the potential for using rechargeable batteries to power the system. By developing an energy-efficient solution, this research aims to lower the energy costs associated with oil transportation, enhancing the sustainability of pipeline operations. The ultimate goal is to create a cost-effective, reliable, and environmentally friendly method to prevent and clear wax blockages, improving oil flow while reducing operational disruptions and energy consumption.	fluid mechanics	Both: Theoretical (Computational or Modelling) + Experimental	Degree in Chemical Engineering, Materials Science, Mechanical Engineering, Physics, or a related field. Basic knowledge of solid mechanics and fluid dynamics Training provided for specific experimental and modeling techniques An enthusiasm for developing and creating new devices, along with a passion for exploring innovative solutions, is essential.
	FA-20 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth and Abhijit Majumdar	Investigating the Effect of Gel Deformation on Cell Migration	This PhD project will investigate how the deformation of gels influences the migration of stem cells, specifically examining how mechanical cues, such as changes in gel shape or stiffness, affect cell movement. In previous work, it has been observed that stem cells migrate from regions of high to low loss modulus in soft materials. The research will explore how different types of gel deformation—such as compression, stretching, and shear—impact the migration and behavior of stem cells. The candidate will be involved in creating and refining experimental setups to deform gels in various ways, simulating real-life conditions that stem cells might encounter in biological environments, such as during tissue development or injury repair. The goal is to understand how mechanical properties of the environment influence stem cell dynamics, which can be applied to tissue engineering, regenerative medicine, and cell-based therapies.	Cell Migration	Both: Theoretical (Computational or Modelling) + Experimental	The candidate should have a background in biomedical engineering, bioengineering, materials science, or a related field. While prior experience with gel mechanics or stem cell biology is not required, the candidate should be eager to learn about these areas. The project will involve experimental work, including gel preparation, stem cell culture, and developing methods to induce gel deformation. Strong problem-solving skills and an interest in building and developing new experimental setups will be essential.

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	FA-21 (JS)	jyotiseth@iitb.ac.in	Jyoti R Seth and Vinay Juvekar	Self-Assembly of 3D Structures from 2D Particles: From Design to Application	Creating three-dimensional (3D) materials from two-dimensional (2D) particles like graphene sheets opens up exciting possibilities in areas like energy storage, catalysis, filtration, and structural materials. This PhD project aims to understand and optimize how 2D sheet-like particles can be transformed into robust and functional 3D structures. You'll explore how chemical reduction methods, interaction forces, and assembly dynamics affect the final material properties—like strength, flexibility, and surface area. To better understand the self-assembly process, you'll also build and test a model experimental system using 3D-printed particles embedded with magnets to mimic how 2D particles interact in real systems.	self-assembly	Both: Theoretical (Computational or Modelling) + Experimental	Skills You'll Develop during this PhD Materials synthesis and assembly techniques Characterization tools (e.g., SEM, TEM, XRD, BET, Raman spectroscopy) Understanding of colloidal and nanoscale interactions Design and execution of physical models (e.g., using 3D printing) Experimental data analysis and mechanical testing Simulation or modeling of self-assembly processes
	FA-22 (PS)	p.sunthar@iitb.ac.in	P Sunthar	Optimizing Lithium-Ion Battery Cycles for Maximised Lifetime and Safety	The performance and lifespan of Lithium Ion Batteries (LIBs are limited by the irreversible degradation in a battery cell. This project aims to understand the processes at the cell level to obtain optimal charging and discharging protocols for various load demands and renewable energy production rates. We will employ tools such as Discrete Element Method (DEM) and physics-assisted machine learning (PAML) and physics-informed neural networks (PINN) in an attempt to solve the problem. https://www.che.iitb.ac.in/phd-ta-topic/optimizing-lithium-ion-battery-cycles-maximised-lifetime-and-safety	Modelling	Theoretical / Computational / Modelling	Chemical engineering, Physics, Python programming
	FA-23 (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-24 (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

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	FA-25 (RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Gravity-driven device for removal of microorganisms, metals and microplastics from water	We have already developed a working prototype for killing and removal of E. coli from water. It is based on our synthesized nanocomposite, made of Ag-Cu nanoparticle impregnated on granular activated carbon and packed into a column, which is driven by gravity-head of the water column. Consequently, it can continuously disinfect water in absence of electricity, by the action of nanoparticles on the bacteria. In the current project, the aim is to further study the removal of virus, heavy metals and microplastics, by the same or related class of nanocomposites, as these are all critical contaminants present in water. The final outcome could be a modular water treatment device, usable for household drinking water needs, by combining concepts of adsorption, reaction engineering, fluid flow and functional design principles to make a energy self-sufficient device. The work is mostly experimental with reasonable scope of modeling, if the student is interested. They get to work and learn in a multidisciplinary team of life sciences and engineering students, contributing to the overall goal of the project.	Water treatment by nanoparticles	Experimental	Chemical, Environmental, Materials Engg., Microbiology, Chemistry, Life Sciences
	FA-26 (RT)	rochish@che.iitb.ac.in	Rochish M Thaokar	Experiments and phenomenonlogical as well as physics informed ML modeling of biomemetic excitable and unexcitable cells (GUVs)	Our group works on unexcitable and excitable biomemetic cells, made up of Giant Unilamellar Vesicles using experiments, theory and simulation as well. TThe objective in these works is to understand the complex multiphysics in these systems involving hydrodynamics, electrostatics and kinetics and membrane mechanics. In the past, we have conducted studies on electroporation and excitation of these systems. The proposed work will extend these studies for relevance to realising bio-memetic cells suitable for electroporation physics as well as extending phenomenological models to physics informed ML models. The work will involve all three components, experiments, theory and simulations. Recent references: Compound giant unilamellar vesicles as a bio-mimetic model for electrohydrodynamics of a nucleate cell R Kumar, R Chakrabarti, RM Thaokar Soft Matter 20 (35), 6995-7011, 2024 Electrohydrodynamics of vesicles and capsules K Priti Sinha, S Das, RB Karyappa, RM Thaokar, Langmuir 36 (18), 4863-4886, 2020	Biophysics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering, Physics, Biotechnology,
	FA-27 (RT)	rochish@che.iitb.ac.in	Rochish M Thaokar	Novel electric field based physics for inventing novel sustainable processes for chemical industries and intensifying existing unit operations	Our group has been working on intensifying existing unit operations such as electrodesalters in oil refineries, and inventing new electric field based processes such as in indoor air cleaners. The approach is to understand and invent novel electric field based physics through hydrodynamic and chemical effects, and then employ then to devise new sustainable unit operations. The PhD will involve further progressing our research in electrodesalters and air cleaners but also explore newer unit operations, by conducting research in the fundamentals of electrohydrodynamics. The work will involve all three components, experiments, theory and simulations. Recent references: Electrocoalescence of a pair of conducting drops in an insulating oil, V Anand, S Roy, VM Naik, VA Juvekar, RM Thaokar, Journal of Fluid Mechanics 859, 839-850, 2019 Mitigating noncoalescence and chain formation in an electrocoalescer by electric field modulation, R Hasib, V Anand, VM Naik, VA Juvekar, RM Thaokar, Industrial & Engineering Chemistry Research 61 (46), 17145-17155, 2022	Process Intensification	Both: Theoretical (Computational or Modelling) + Experimental	Physics, Mechanical, Chemical
	FA-28 (SRJ)	srjadhav@iitb.ac.in	Sameer Jadhav	Design, analysis and control of flow in microfluidic networks	Microfluidics technology has been seen to have great potential in lab-on-a-chip applications including chemical analysis and diagnostics. One may be able to control flow direction and flow rate as well as concentration of solutes in specific branches of the microfluidic network for certain designs of the network and the resistance to flow in each branch of the network. In this project we explore several designs and optimize geometric and flow parameters of the microfluidic network for desired flow and concentration patterns. The work is in collaboration with Prof. Ganesh Viswanathan.	Network Analysis	Theoretical / Computational / Modelling	B.Tech/M.Tech in Chemical Engineering, Mechanical Engineering or Biotechnology (with fluid mechanics subject).
	FA-29 (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-30 (SMe)	sarika@che.iitb.ac.in	Sarika Mehra	Synthetic Biology tools to create host cell lines for production of recombinant proteins	A large number of therapeutics used to treat a range of diseases are recombinant proteins, that require mammalian cells as a host for their commercial production. Chinese hamster ovary (CHO) cell lines are the most preferred host cells for the production of a variety of biotherapeutics ranging from interferons to antibodies. Similarly, many vaccine candidates, such as the receptor binding domain of the SARS-COV2 are also produced in mammalian cells due to their glycosylation. The increasing demand to treat a variety of diseases has necessitated the need to increase the overall productivity of these therapeutic proteins. Further, the pandemic highlighted the need to shorten the clone development timelines for rapid production of antibodies and vaccine candidates. In this project, we will create a panel of cell lines based on genetic engineering targets identified in our lab and evaluate these cell lines for increased secretion of model recombinant proteins and Monoclonal Antibodies.	systems and synthetic biology	Experimental	Biotechnology/Molecular Biology/Chemical Engineering. Experience in cell culture or cloning will be a plus.
	FA-31 (SMe)	sarika@che.iitb.ac.in	Sarika Mehra	Upstream Process development for recombinant therapeutics including MABs and vaccine subunits		biochemical engineering	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering/Biotechnology
	FA-32 (SyD)	sayantan.dutta@iitb.ac.in	Sayantan Dutta	Cell Division: A sphere packing problem	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	1. Engineering/Physics/Physical Chemistry training 2. Stat Mech training would be a plus

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	FA-33 (SD)	sonali.das@iitb.ac.in	Sonali Das	Catalyst development for applications in storage of green hydrogen in the form of liquid hydrogen carriers.	This project aims at the development of new catalysts and catalytic processes for the conversion of hydrogen into liquid hydrogen carriers and vice versa, which is an important step towards establishing a sustainable green hydrogen economy. The work would entail development of new catalyst materials, characterization, testing catalyst performance in reactors and detailed kinetic studies for green H2 applications.	Catalysis, Green Hydrogen, Sustainability	Experimental	
	FA-34 (SD)	sonali.das@iitb.ac.in	Sonali Das	Catalyst and Process development for Plasma-catalytic Methane Valorization	This project aims at development of a lab-scale integrated plasma-catalytic reactor system incorporating novel catalysts for methane conversion to value-added higher hydrocarbons. Conversion of waste methane such as landfill gas etc. into value-added higher hydrocarbons is a highly desirable process in the context of environmental sustainability and greenhouse gas emissions. This project aims to use novel "plasma-catalysis" to accomplish this challenging conversion process. The work will entail development of new catalysts, characterization, catalyst testing. and design of plasma-catalytic hybrid reactors.	Catalysis, Nanomaterials, Sustainability	Experimental	
	FA-35 (SD)	sonali.das@iitb.ac.in	Sonali Das	Development of novel photothermal catalysts for sustainable carbon dioxide conversion using solar energy.	Converting CO2 into synthetic fuels and chemicals using sunlight as the sole energy source holds tremendous prospects for establishing a sustainable carbon-neutral economy. This project aims at developing novel photothermal catalysts to convert CO2 into value-added chemicals by harvesting both heating and optical properties of solar energy. The work will involve development of new nanomaterials (such as MOFs, core-shell catalysts), advanced material characterization, and photothermal reaction and reactor design.	Catalysis, nanomaterials, sustainability.	Experimental	
	FA-36 (SV)	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay	Machine Learning to Predict Stable Electrocatalysts Faster	When designing new materials, like next-generation batteries, catalysts, semiconductors, or systems for green hydrogen generation, researchers need to understand how atoms arrange themselves into stable configurations. This requirement is especially important in electrochemical reactions, such as those used in water splitting for hydrogen production, where the efficiency and stability of materials directly determine performance and cost. Finding these stable atomic structures is like solving a massive 3D puzzle with billions of possibilities. Traditionally, we've used physics-based search methods (like basin hopping or minima hopping) to explore the energy landscape of materials, hunting for the most stable configurations. While reliable, these methods are computationally expensive and slow, limiting the scale and speed at which we can create new materials. Now, there is an alternative approach: generative machine learning (ML). Instead of checking every possibility one-by-one, ML models learn from a database of known stable structures (generated using density functional theory, a simulation method). Architectures such as autoencoders, generative adversarial networks, and transformers can then generate new, stable structures much faster. What you will do in the project: (1) Develop state of the art machine learning methods from scratch (2) Compare traditional search methods with the machine learning models you develop (3) Perform large scale simulations on the fastest and most advanced high-performance computing clusters in India (4) Develop a nuanced understand of what types of problems machine learning is (or isn't) good at solving in chemical engineering Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group: https://www.che.iitb.ac.in/web/faculty/sv/	machine learning for science and engineering	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering or Chemistry and Physics who are curious about clean energy, catalysis, and computational modeling. You don't need prior experience in DFT or machine learning, just a willingness to learn.
	FA-37 (SV)	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay	Understanding Catalyst Surfaces Using Quantum Mechanical and Analytical Models	This project focuses on using theory and computer simulations to understand how and why catalysts work, with the goal of designing better ones for important chemical and electrochemical reactions. We use theoretical models and simulations to study how molecules interact with the surfaces of catalysts. These surface interactions control how fast or efficiently a reaction occurs. For example, if molecules binds too weakly to the surface, the catalyst won't activate them. If they bind too strongly, the surface can get poisoned. The key is to find the right balance. We study these interactions using two main approaches: (1) Quantum mechanical simulations, such as density functional theory (DFT), which help us calculate how atoms and electrons behave on catalyst surfaces. Analytical models, like the Newns-Anderson model and related methods, which give us physical insight into how a material's electronic structure (such as the position of its d-band) affects reactivity. What you will do in this project: (1) Use density functional theory (DFT) to simulate how molecules bind and react on catalyst surfaces. (2) Learn and apply analytical models such as the Newns-Anderson model to understand how electronic structure controls catalytic activity. (3) Extend these models to include more realistic effects, such as electric fields, co-adsorption of molecules, and complex alloy surfaces. (4) Compare predictions from simple models with detailed quantum mechanical simulations to build physical intuition. (5) Identify trends and design principles that can help develop new catalysts for reactions like green hydrogen production and electrochemical energy conversion. By combining first-principles simulations with physics-based models, this project aims to develop a general theory of how surface chemistry works. This understanding can guide the design of new catalysts for processes like green hydrogen production, CO_2 reduction, or ammonia synthesis. Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group: https://www.che.iitb.ac.in/web/faculty/sv/	Catalysis	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering or Chemistry and Physics who are curious about clean energy, catalysis, and computational modeling. You don't need prior experience in DFT or machine learning, just a willingness to learn.

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	FA-38 (SV)	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay	Bridging Atomistic Simulations and Machine Learning: Smarter Ways to Model Chemical Reactions	Understanding how atoms behave during chemical reactions is key to solving big challenges in fields like catalysis, energy storage, and electrochemistry. Traditionally, we use accurate but computationally expensive methods like density functional theory (DFT) to simulate these reactions. While powerful, DFT can only handle small systems and short time scales. To study real-world reactions, which happen over longer times and larger systems, we need faster tools. That's where machine learning models are particularly effective. By training machine-learned interatomic potentials (MLIPs) on atomic data, we can get DFT-level accuracy at a fraction of the cost. For these models to be reliable, they must be trained on the right kinds of atomic structures. This project explores smart ways to choose those structures, making the models both faster and more accurate. What you will do in this project: (1) Learn how machine learning models can predict atomic behavior in chemical reactions, using only a small amount of high-quality simulation data. (2) Explore two powerful selection strategies: Bayesian methods – to estimate the model's uncertainty and guide where more data is needed. Committee methods with neural networks – where a team of models "vote" on which data will help improve accuracy. (3) Apply and test these methods on example systems like metal oxides and water–ion mixtures that are relevant to real applications in electrocatalysis. You will run your calculations on fast computers in high performance computing clusters in India. Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group: https://www.che.iitb.ac.in/web/faculty/sv/	machine learning for science and engineering	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering or Chemistry and Physics who are curious about clean energy, catalysis, and computational modeling. You don't need prior experience in DFT or machine learning, just a willingness to learn.
	FA-39 (SV)	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay / Ojus Mohan	Designing Better Catalysts by Combining Industrial Data and Atomistic Simulations with Machine Learning	Chemical industries rely on catalysts to make reactions faster, more efficient, and more sustainable. However, designing new catalysts is often a slow, trial-and-error process. In this project, we're taking a new approach. We will combine industrial reactor data with atomic-level simulations to speed up catalyst design. We will use density functional theory (DFT). DFT is a type of quantum mechanical simulation tool that lets us predict how atoms and electrons behave in chemical systems. Using DFT, we can calculate how strongly molecules bind to a catalyst surface and what reaction barriers need to be overcome. While DFT gives us detailed information at the atomic level, it is limited in length and time-scale. On the other hand, industrial data (temperature, pressure, conversion, and selectivity) tells us how catalysts behave in full-scale reactors, but doesn't tell us what happening at the atomic level. Our goal is to connect these two pictures. We'll use generative machine learning models to learn patterns from both kinds of data and suggest new catalysts and optimal reaction conditions. What You Will Do in the Project: (1) Understand how DFT calculations are performed (2) Work with industrial reactor datasets to understand real-world catalytic performance (3) Train machine learning models that connect atomistic and industrial-scale data (4) Generate new catalyst ideas and reaction environments based on model predictions (5) Bridge fundamental science with real chemical engineering applications Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group: https://www.che.iitb.ac.in/web/faculty/sv/	generative machine learning	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering who are curious about heterogeneous catalysis and machine learning. You don't need prior experience in DFT or machine learning, just a willingness to learn.
	FA-40 (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-41 (SS)	saini@che.iitb.ac.in	Supreet Saini	From genes to genomics, and beyond.	Units of inheritance (or genes) were first proposed by Mendel in 1860s. However, the chemical basis of genes was not understood for another 100 years. This means that the definition and understanding of the word "gene" has undergone radical transitions. In the era of genomics, the relative role of a single gene is again being redefined and understood. In this project, we will study the transition from genes to genomics, and what does the future of evolutionary biology holds.	Evolutionary biology	Theoretical/Computational	Strong interest in evolutionary biology and history.
	FA-42 (SS)	saini@che.iitb.ac.in	Supreet Saini	Role of epistasis in dictating evolution of SARS CoV-2	SARS CoV-2 variants keep getting detected. However, does evolution of newer viral variants follow certain rules? How do the mutations that have already occurred and spread in populations dictate the future evolution of the virus? In this work, we will study the sequence evolution of SARS CoV-2 virus variants, and develop a framework to understand how epistasis constrains and/or facilitates evolution.	Evolution	Theoretical/Computational	Interest in Evolutionary Biology; Prior experience/comfort in coding.

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	FA-43 (SwB)	swaticb@iitb.ac.in	Swati Bhattacharya	Using computer simulations to find a cure for diabetes	As of 2025, approximately 9.6% of India's population aged 20 to 79 years is affected by diabetes, according to World Bank data. In absolute numbers, this translates to over 212 million people, making India the country with the highest number of individuals living with diabetes globally. The prevalence is higher in urban areas (11.2%) compared to rural areas (5.2%), and a significant portion of cases remain undiagnosed. Intrinsically disordered proteins (IDPs) are deeply involved in the pathogenesis of type 2 diabetes mellitus (T2DM) due to their flexible structures, which enable them to interact with multiple molecules and regulate key biological processes. Proteins such as IRS1, IRS2, and IRS4, which mediate insulin signaling, are highly disordered and play crucial roles in glucose metabolism. Their disordered regions often serve as hubs for protein-protein interactions and post-translational modifications, which are essential for proper insulin function. Dysregulation of these IDPs can impair signaling pathways, contributing to insulin resistance and hyperglycemia. Understanding the functional roles of IDPs in diabetes provides insights into novel therapeutic targets, potentially paving the way for innovative drug discovery aimed at stabilizing or modulating their activity. Using state-of-the-art computer simulations we will reveal structural details of IDPs involved in the pathogenesis of T2DM, identify temporary folds or binding sites, that might contribute to diabetes when disrupted. By understanding IDPs' dynamic behavior, researchers can design drugs that stabilize or block their harmful interactions—opening doors to treatments that were previously impossible to develop.	Computational Biophysics	Theoretical / Computational / Modelling	Students from chemical engineering, chemistry, physics, engineering physics, Biotech/BioEngineering.
	FA-44 (SwB)	swaticb@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.
	FA-45 (VG)	venkatg@iitb.ac.in	Venkat Gundabala	Development of nanomaterial-microparticle composites for sensing applications using microfluidics	Polymeric microparticles embedded with nanomaterials have applications in drug delivery, tissue engineering, biosensing, and catalysis. Existing conventional methods to synthesize these materials suffer from drawbacks such as complex fabrication, lack of control over size, non-uniform encapsulation/coating, etc. Microfluidics, with its superior control over process parameters, is an ideal alternative to existing fabrication techniques. In this project, the student will a) design and fabricate microfluidic devices for synthesis of nanomaterial-microparticle composites, b) optimize the process parameters for controlling the size, composition, and morphology of these composites, and c) test them for sensing applications. The project is predominantly experimental in nature. Reference Wang, W. E. I., Zhang, M. J., & Chu, L. Y. (2014). Functional polymeric microparticles engineered from controllable microfluidic emulsions. Accounts of chemical research, 47(2), 373-384.	Microfluidics	Experimental	Chemical engineering, Nanotechnology, Materials engineering, Experimental background
	FA-46 (VG)	venkatg@iitb.ac.in	Venkat Gundabala (Supervisor) and Mahesh Tirumkudulu (Co-supervisor)	Biodegradable Antibacterial Implant for Localised Prevention and Management of Bone Infections	Biodegradable antibacterial systems offer a promising localised drug delivery strategy for the prevention and management of osteomyelitis. Composed of biocompatible polymers or composites, these systems enable sustained, site-specific antibiotic release, maintaining therapeutic levels at the bone–tissue interface while minimising systemic toxicity. The architecture of the composite supports high drug loading and cellular infiltration, promoting both antimicrobial efficacy and tissue regeneration. Importantly, the combination of controlled antibiotic release and intrinsic antibacterial properties prevents bacterial adhesion and biofilm formation, mitigating colonisation at the implantation site. The complete biodegradation into non-toxic byproducts eliminates the need for surgical removal, presenting a clinically effective and patient friendly solution. In this project, the student will develop biodegradable implants for localised delivery of antibiotics to bone tissue, characterize their biodegradability, mechanical strength, release kinetics, and perform in vitro experiments to test their efficacy in preventing microbial growth. Reference Nie, B. E., Huo, S., Qu, X., Guo, J., Liu, X., Hong, Q., & Yue, B. (2022). Bone infection site targeting nanoparticle-antibiotics delivery vehicle to enhance treatment efficacy of orthopedic implant related infection. Bioactive Materials, 16, 134-148.	Healthcare	Experimental	Chemical engineering, Biotechnology, Experimental experience

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	List of TA topics that will be available for PhD students selected under TA cetegory in May 2025 admission round. All candidates who have applied under TA/RA/FA category are eligible to opt for TA choice.							
	TA-A	achatter@iitb.ac.in	Abhijit Chatterjee	Combined experimental and computational analysis of coupled multiphase flow dynamics and electrocatalytic reactions in alkaline water electrolyzers	An alkaline water electrolyzer (AWE) is used to produce hydrogen and oxygen gases by splitting water molecules. This technology is widely used for industrial-scale hydrogen production and is considered a key component in the transition to green energy. Efforts are underway at IITB to develop a 10 kW AWE. The electrolyzer will consist of two electrodes (a cathode and an anode) immersed in a liquid alkaline (KOH/NaOH) electrolyte. At the cathode, water molecules are reduced, producing hydrogen gas. At the anode, hydroxide ions are oxidized, generating oxygen gas. A key challenge is that the growth and coalescence of gas bubbles at the electrodes causes the formation of a bubble curtain which affects the electrochemical reactions and ohmic drop. Detailed models for capturing this complex phenomenon are lacking. The main aim of the project is to develop integrated models that account for: (i) electrochemical reactions at rough, porous electrode surfaces leading to gaseous products, (ii) bubble formation/pinning characteristics, (iii) nucleation, growth, and coalescence of gas bubble, and (iv) fluid dynamics model of release of gas bubbles. Such a development will help improve the current AWE design. The student will be co-advised by Profs. Abhijit Chatterjee, Partha Sarthi Goswami and Ratul Dasgupta.	Fluid dynamics, catalysis	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering
	TA-B	amol.subhedar@iitb.ac.in	Amol Subhedar	Capillary-Driven Dynamics of Microparticles with Contact Angle Hysteresis at Fluid Interfaces	This project studies the dynamics of microparticles connected by liquid bridges, focusing on how capillary forces and contact angle hysteresis affect their motion and collective behavior. Particles at deformable fluid interfaces generate long-range interactions that can lead to clustering, migration, or self-assembly. The Lattice Boltzmann Method will be used to simulate the coupled fluid-interface-particle system, with emphasis on modeling hysteresis and moving contact lines. The project will examine how hysteresis influences pattern formation and symmetry breaking. Applications include microfluidics, emulsions, and interfacial self-assembly.	Computational fluid mechanics	Theoretical / Computational / Modelling	Any Engineering descipline
	TA-C	amol.subhedar@iitb.ac.in	Amol Subhedar	Modeling Two-Phase Flow with Phase Change Using Lattice Boltzmann:	The Lattice Boltzmann Method (LBM) is increasingly preferred for solving fluid dynamics problems, especially due to its ability to handle wetting and no-slip boundary conditions in complex geometries. This project aims to develop a two-phase, phase-change model using a multi-component LBM framework. A key challenge is ensuring that the macroscopic behavior aligns with the kinematic conditions at the fluid–fluid interface, which will be addressed through multi-scale analysis. The project includes modifying an existing C++ LBM code and will be applied to the problem of droplet evaporation, characterized by high density contrasts and wetting effects.	Computational Fluid Mechanics	Theoretical / Computational / Modelling	Any Engineering discipline
	TA-D	a.sarkar@iitb.ac.in	Arindam Sarkar	Electrosynthesis of hydrogen peroxide	This project focuses on the design and development of advanced catalysts and electrochemical cell configurations to enable efficient, selective, and sustainable electrosynthesis of hydrogen peroxide (H_2O_2). Hydrogen peroxide is a valuable green oxidant with wide-ranging applications in environmental remediation, chemical manufacturing, and healthcare. However, traditional methods of H_2O_2 production, such as the anthraquinone process, are energy-intensive and centralized, posing environmental and economic limitations. The proposed research aims to address these challenges by investigating electrochemical pathways for in situ H_2O_2 generation, particularly via the two-electron oxygen reduction reaction ($2e^-$ ORR). Key goals include (a) Synthesizing and characterizing transition-metal-based or alloy catalysts with high selectivity toward the $2e^-$ ORR pathway. (b) fabricating tailored electrodes, including gas diffusion electrodes and porous structures, to support efficient mass transport and electron transfer. Electrochemical cells—ranging from H-type cells to flow cells—will be developed and optimized to enhance H_2O_2 productivity and scalability, and (c) Systematic testing of catalyst-electrode-cell systems under various operating conditions (e.g., electrolyte composition, pH, applied potential, temperature) to maximize Faradaic efficiency, H_2O_2 concentration, and long-term stability. The project is experimental in nature. (1) Shi, X.; Back, S.; Gill, T. M.; Siahrostami, S.; Zheng, X. Electrochemical Synthesis of H2O2 by Two-Electron Water Oxidation Reaction. Chem 2021, 7 (1), 38–63. https://doi.org/10.1016/j.chempr.2020.09.013. (2) Perry, S. C.; Pangotra, D.; Vieira, L.; Csepei, L.-I.; Sieber, V.; Wang, L.; Ponce de León, C.; Walsh, F. C. Electrochemical Synthesis of Hydrogen Peroxide from Water and Oxygen. Nat Rev Chem 2019, 3 (7), 442–458. https://doi.org/10.1038/s41570-019-0110-6.	Electrochemistry	Experimental	
	TA-E	a.sarkar@iitb.ac.in	Arindam Sarkar	Investigations on electrochemical CO2 reduction to formate and other C1/C2 chemicals	This is an experimental research project centered on the electrochemical reduction of carbon dioxide (CO_2) into formate or other high-value chemical products (1,2). The work will explore the design, synthesis, and application of metal and alloy-based catalysts, with a particular emphasis on their integration into gas diffusion electrodes (GDEs). These electrodes will be tested and optimized within a novel electrochemical setup, primarily utilizing a two-electrode flow cell configuration, although a three-electrode system may also be employed for more detailed mechanistic studies. The experimental tasks will involve the synthesis of nanoparticles and catalytic materials, followed by comprehensive physico-chemical and electrochemical characterization. Techniques may include, but are not limited to, transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and cyclic voltammetry (CV). The products will be analyzed using HPLC/GC. Although prior experience in electrochemistry is not a prerequisite, the student is expected to develop a strong foundation in advanced electroanalytical techniques and physical characterization methods over the course of the project. This experience will be integral to understanding catalyst performance and reaction mechanisms in CO_2 electroreduction systems. The project is experimental in nature. (1) Al-Tamreh, S. A.; Ibrahim, M. H.; El-Naas, M. H.; Vaes, J.; Pant, D.; Benamor, A.; Amhamed, A. Electroreduction of Carbon Dioxide into Formate: A Comprehensive Review. ChemElectroChem 2021, 8 (17), 3207–3220. https://doi.org/10.1002/celc.202100438. (2) Giri, S. D.; Mahajani, S. M.; Suresh, A. K.; Sarkar, A. Electrochemical Reduction of CO2 on Activated Copper: Influence of Surface Area. Materials Research Bulletin 2020, 123, 110702. https://doi.org/10.1016/j.materresbull.2019.110702.	Electrochemistry	Experimental	

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	TA-F	a.sarkar@iitb.ac.in	Arindam Sarkar	Investigating the Underlying Unity of Chemical and Electrochemical Processes	It has been reasonably established that catalytic chemical oxidation and electrochemical oxidation are not fundamentally different or unrelated processes. Rather, they appear to be different manifestations of the same underlying electrochemical mechanism. In this context, the project aims to develop a more unified framework for comparing chemical and electrochemical oxidation pathways, building on the work conducted by previous students. The selected candidate will be expected to extend this research and rigorously investigate the equivalence between chemical and electrochemical oxidation mechanisms, particularly in non-aqueous systems. A key focus will be on understanding the role of dopants and poisons in modulating these pathways. At a later stage, the project may also involve the synthesis of nanoparticulate catalysts. While prior experience in electrochemistry is not mandatory, the student should possess a strong interest in analytical electrochemistry and detailed analysis of current–voltage behavior and reaction mechanisms. The project is experimental in nature with a small degree of modelling. (1) Chauhan, N. L.; Dameera, V.; Juvekar, V. A.; Mahajani, S. M.; Suresh, A. K.; Sarkar, A. Correlation of Chemical and Electrochemical Catalysis-Importance of Half Reactions: The Case of Catalytic Oxidation of Ferrous Sulfate by Molecular Oxygen. Journal of The Electrochemical Society 2018, 165 (5), H196–H204. (2) Chauhan, N. L.; Juvekar, V. A.; Sarkar, A. Oxidation of Ethylene Glycol: Unity of Chemical and Electrochemical Catalysis. Electrochemical Science Advances 2022, 2 (6), e2100092.	Electrochemistry	Experimental	
	TA-G	amalani@IITB.ac.in	Ateeque Malani	Design and Synthesis of Porous Materials for natural gas storage	Natural gas (NG) has very low energy density compared to diesel and petrol, hence NG is often compressed or liquefied to increase it. The process of compression or liquefaction are often costly and has serious safety issues. An alternative is to adsorb NG in porous materials. The aim of this project is to use computational approach to design novel porous materials and synthesise them using experimental approach.	Natural Gas, Energy, Porous Materials	Both: Theoretical (Computational or Modelling) + Experimental	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
	TA-H	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-I	amalani@IITB.ac.in	Ateeque Malani	Simulation studies of enhanced oil recovery	With increase in energy demand, the requirement of crude oil is expected to increase worldwide. The current oil production rates are significantly affected due to depletion of oil from existing reservoirs. Thus to increase production rates, enhanced oil recovery approach needs to be adopted. However, current approach is mostly heuristic and practise based. The aim of this project is use chemical engineering fundamentals to study enhance oil recovery process to design guidelines.	Energy, Oil recovery	Theoretical / Computational / Modelling	Enthusiastic student with background in Chemical, Mechanical, Material Science, Chemistry, Physics, and passion for coding
	TA-J	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-K	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-L	guruswamy@iitb.ac.in	Guruswamy Kumaraswamy	Sustainable bio-derived polymers: Structure-property relations	Bioderived polymers represent a possible solution to the problem of plastic pollution. However, to replace the dominant synthetic polymers such as polyethylene and polypropylene, these polymers will need to have suitable balance of properties. The properties of polymers are governed by their (often non-equilibrium) structure. This project will aim at developing suitable bioderived polymer substitutes (such as cellulosics, algal polysaccharides or polyhydroxyalkanoates) for specific circular applications. This is primarily experimental and will involve rheology, thermal analysis, scattering and solid property measurements. There is also a possibility of collaboration with industry partners.	Sustainable bioderived polymers	Experimental	No specific background
	TA-M	guruswamy@iitb.ac.in	Guruswamy Kumaraswamy	Formation of micro and nanoplastics	The annual global production of synthetic plastics is of the order of 400 million tons. A majority of these materials are improperly disposed and undergo environmental degradation. This results in the formation of particulate pollutants, micro and nanoplastics. Understanding how plastics degrade to form such pollutants is an area of great contemporary importance. In this project, we will explore the fundamental principles that guide the degradation of plastics and how this results in the formation of micro and nanoplastics. This is primarily an experimental project, and will involve a wide swathe of characterization techniques, that are available in the institute. Interested students can refer to some recent papers from our group in this area (nature.com/articles/s41467-025-58233-3 and https://doi.org/10.1039/D5SM00074B)	Microplastics	Experimental	No specific background
	TA-N	hnanavati@iitb.ac.in	Hemant Nanavati	Accurate Molecular Models for Real Polymers	We develop compact, closed form, but accurate molecular models as well as elasticity relationships for real polymers, incorporating structural aspects. The applications include synthetic (e.g., those used as matrix for solid propellant) as well as high performance Bio-sourced polymers.	Polymer Physics	Theoretical / Computational / Modelling	Chemical Engg/Chemistry/Physics/ Materials Science/Polymers/ Knowledge of coding
	TA-O	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of 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.	Biopolymer Physics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engg/Chemistry/Physics/ Materials Science/Polymers/ Knowledge in coding
	TA-P	jyotiseth@iitb.ac.in	Jyoti R Seth	Why Do Like-Charged Polymers Stick Together? Exploring Polyethylenimine in Acidic Water	Normally, materials with the same charge repel each other. But in some cases—like with the polymer polyethylenimine (PEI) in acidic water—they actually come together and form fascinating structures. This PhD project will use computer simulations (and maybe some expeirments) to figure out why this happens. You'll dive into the tiny world of molecules to see how acid levels, ions, and water molecules affect the way these polymers behave. The results could help improve things like gene delivery in medicine. If you're into soft matter, modeling, simulations, or nanoscale interactions—this is for you!	self assembly	Both: Theoretical (Computational or Modelling) + Experimental	Skills You'll Need or Develop: Molecular dynamics simulations (e.g., GROMACS, LAMMPS, or similar), Basic programming (Python or similar for data analysis and scripting), Understanding of thermodynamics and intermolecular forces, Data visualization and analysis, understanding of soft matter or nanomaterials No worries if you don't have all of these yet—this PhD is designed to help you build them

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	TA-Q	jyotiseth@iitb.ac.in	Jyoti R Seth	Multiscale Modeling of Crystallization Dynamics	This PhD project aims to explore how crystals grow in solutions. The research will use computer simulations along with a few carefully designed experiments to study how crystals start to form, how fast they grow, and how certain chemicals—called additives—can help or slow down this process. By combining models that look at both small-scale (molecular) and larger-scale behaviors, the project will give a clearer picture of what controls crystal growth. These insights are important for improving processes in medicine, materials design, and electronics.	Crystallisation	Both: Theoretical (Computational or Modelling) + Experimental	The ideal candidate should have a background in chemistry, chemical engineering, physics, materials science, or a related field, and a strong interest in learning new techniques. During the PhD, the candidate will be trained in: Computer modeling and multiscale simulation methods Basic programming (e.g., Python, MATLAB) Experimental techniques related to crystallization Data analysis and scientific communication Strong problem-solving skills and curiosity about molecular processes are highly valued. No prior experience in simulations or crystallization is mandatory as requisite training will be provided as part of the project.
	TA-R	jyotiseth@iitb.ac.in	Jyoti R Seth	Modeling the Dynamics and Flow Behavior of Non-Newtonian Fluids	This PhD project will study how complex fluids behave when they flow and how certain additives—like polymers, nanoparticles, and surfactants—can change their flow properties. Using computer simulations and special programs, the research will look at how factors like temperature, pressure, and concentration affect fluid flow. The aim is to create a model that helps design better materials and additives for improving the performance of fluids in industries like oil, medicine, and materials science.	Fluid mechanics	Both: Theoretical (Computational or Modelling) + Experimental	The ideal candidate will have a background in chemical engineering, physical chemistry, materials science, or a closely related field. During the PhD, the candidate will gain expertise in: Fluid dynamics, Molecular dynamics simulations, utilizing platforms like GROMACS or LAMMPS Computational modeling of rheological properties Advanced data analysis, visualization techniques, and statistical modeling Fundamental principles of rheology and material behavior in complex fluids Scientific writing, communication, and presentation skills Prior experience with computational simulations or programming is advantageous but not required—full training will be provided throughout the PhD.
	TA-S	jyotiseth@iitb.ac.in	Jyoti R Seth	Simulating the Elasticity of Soft Materials for Biomedical and Environmental Applications	This PhD project will explore how the size, shape, and connectivity of nanoparticles or microparticles influence the strength, flexibility, and performance of materials such as tissue engineering scaffolds, clays, hydrogels, and oleogels. By using advanced computer simulations, we will analyze how these particles interact to form networks, how their connectivity impacts material properties, and how the networks respond under stress. A few experiments may also be performed to validate and complement the simulation results. The aim is to develop a predictive tool that enables the design of materials with optimal strength, flexibility, and network connectivity. This research will be valuable for industries ranging from biomedical engineering (e.g., tissue scaffolds), pharmaceuticals (e.g., drug delivery systems), materials science (e.g., hydrogels and oleogels for various applications), and environmental engineering (e.g., clay-based filtration materials).	Colloids and Soft Matter	Both: Theoretical (Computational or Modelling) + Experimental	Degree in Chemical Engineering, Chemistry, Physics, Materials Science, or related field. Familiarity with material characterization (rheology, microscopy), material preparation (hydrogels, oleogels), and mechanical testing is beneficial Computational Skills: Knowledge of computational modeling (particle simulations), coding (Python, MATLAB), and simulation software (e.g., GROMACS, LAMMPS) is a plus; training will be provided. Note: The candidate need not have all the skills listed but will be trained during the course of the project.
	TA-T	jyotiseth@iitb.ac.in	Jyoti R Seth	Energy-Efficient Methods for Clearing Wax Blockages in Crude Oil Pipelines Using Electric Fields	This PhD project will explore innovative methods to clear wax blockages in crude oil pipelines, building on previous research that demonstrates how electric fields can effectively break down wax networks, converting them into low-viscosity liquids that flow more easily. The research will investigate how electric fields can be applied to disrupt wax buildup, ensuring continuous oil flow. Additionally, the project will assess the design of devices to generate these electric fields, the impact of electric fields on wax, and the potential for using rechargeable batteries to power the system. By developing an energy-efficient solution, this research aims to lower the energy costs associated with oil transportation, enhancing the sustainability of pipeline operations. The ultimate goal is to create a cost-effective, reliable, and environmentally friendly method to prevent and clear wax blockages, improving oil flow while reducing operational disruptions and energy consumption.	fluid mechanics	Both: Theoretical (Computational or Modelling) + Experimental	Degree in Chemical Engineering, Materials Science, Mechanical Engineering, Physics, or a related field. Basic knowledge of solid mechanics and fluid dynamics Training provided for specific experimental and modeling techniques An enthusiasm for developing and creating new devices, along with a passion for exploring innovative solutions, is essential.

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	TA-U	jyotiseth@iitb.ac.in	Jyoti R Seth and Abhijit Majumdar	Investigating the Effect of Gel Deformation on Cell Migration	This PhD project will investigate how the deformation of gels influences the migration of stem cells, specifically examining how mechanical cues, such as changes in gel shape or stiffness, affect cell movement. In previous work, it has been observed that stem cells migrate from regions of high to low loss modulus in soft materials. The research will explore how different types of gel deformation—such as compression, stretching, and shear—impact the migration and behavior of stem cells. The candidate will be involved in creating and refining experimental setups to deform gels in various ways, simulating real-life conditions that stem cells might encounter in biological environments, such as during tissue development or injury repair. The goal is to understand how mechanical properties of the environment influence stem cell dynamics, which can be applied to tissue engineering, regenerative medicine, and cell-based therapies.	Cell Migration	Both: Theoretical (Computational or Modelling) + Experimental	The candidate should have a background in biomedical engineering, bioengineering, materials science, or a related field. While prior experience with gel mechanics or stem cell biology is not required, the candidate should be eager to learn about these areas. The project will involve experimental work, including gel preparation, stem cell culture, and developing methods to induce gel deformation. Strong problem-solving skills and an interest in building and developing new experimental setups will be essential.
	TA-V	jyotiseth@iitb.ac.in	Jyoti R Seth and Vinay Juvekar	Self-Assembly of 3D Structures from 2D Particles: From Design to Application	Creating three-dimensional (3D) materials from two-dimensional (2D) particles like graphene sheets opens up exciting possibilities in areas like energy storage, catalysis, filtration, and structural materials. This PhD project aims to understand and optimize how 2D sheet-like particles can be transformed into robust and functional 3D structures. You'll explore how chemical reduction methods, interaction forces, and assembly dynamics affect the final material properties—like strength, flexibility, and surface area. To better understand the self-assembly process, you'll also build and test a model experimental system using 3D-printed particles embedded with magnets to mimic how 2D particles interact in real systems.	self-assembly	Both: Theoretical (Computational or Modelling) + Experimental	Skills You'll Develop during this PhD Materials synthesis and assembly techniques Characterization tools (e.g., SEM, TEM, XRD, BET, Raman spectroscopy) Understanding of colloidal and nanoscale interactions Design and execution of physical models (e.g., using 3D printing) Experimental data analysis and mechanical testing Simulation or modeling of self-assembly processes
	TA-W	mahesh@che.iitb.ac.in	Mahesh Tirumkudulu	Controlled Drug Delivery in Oral Osmotic Tablets: Modelling	The project deals with the mathematical modeling of the drug release process in oral osmotic tablets, which ensures a controlled delivery of the drug inside the body. We have established a tablet manufacturing facility in our lab where we manufacture oral osmotic tablets. As part of the project, We are also studying the in-vitro dissolution process of the tablets. The prospective student would study the flow and mass transfer processes to arrive at a detailed mathematical model of the entire process. We have an ongoing collaboration with Pfizer Inc. and the student would be part of the IITB-Pfizer team studying this problem.	Advanced Drug delivery	Includes both, experiments and modeling	Chemical Engineering, Physics, Chemistry
	TA-X	mahesh@che.iitb.ac.in	Mahesh Tirumkudulu	Biomedical Devices for resource controlled settings	An estimated 700 million Indians live in rural areas with most not having accessing to even basic medical facilities. This leads to deaths despite diseases that are curable and preventable. Around 30% of patients travel more than 30km to seek basic healthcare. Our research group has been working on compact, point-of-care blood cell counter that measures the complete blood count, which is the most basic test to asses one's health. Our goal is to extend the basic framework of the device to other instruments such as electrolyte analyzers that measure the salt content in the blood. The proposed work will involve both experiments and theory with possible application of microfluidics.	Biomedical devices	Includes both, experiments and modeling	Chemical Engg, Physics, Chemistry
	TA-Y	mahesh@che.iitb.ac.in	Mahesh Tirumkudulu	Film formation and Rupture in Drying Polymer Films	The understanding of the film formation process in drying polymer films is critical for a number of applications such as in construction, pharmaceutical Industry and semiconductor. When a thin film of dilute polymer solution is applied on a substrate, the solvent evaporates to concentrate the polymer. With increasing concentration, stresses develop in the film. If the stress exceeds a critical value, the film may rupture or delaminate from the substrate. The critical stress depends on the nature of polymer, solvent, drying rate and the adhesion of the polymer film and the substrate. While there exists a number of studies on the subject, a fundamental understanding of the various phenomena is missing.	Polymer Physics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering and Physics
	TA-Z	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.	Control and Automation	Theoretical / Computational / Modelling	
	TA-AA	mbhushan@iitb.ac.in	Mani Bhushan, Sharad Bhartiya	Causal AI based inferencing of abnormal events in process operations	Machine learning/AI methods for detecting abnormalities are popular in literature. However, to be acceptable to plant operators, it is necessary to not just indicate the abnormality but also explain the causal variables (what is causing the abnormality). This work plans to investigate causal AI ideas to answer this question. In particular, it will look at generating a causal graph from operating data and inferencing in real-time guided by the learnt graph.	Control and Automation	Theoretical / Computational / Modelling	
	TA-AB	mbhushan@iitb.ac.in	Mani Bhushan, Sharad Bhartiya	Autoencoders with ordered variance: static and dynamic models	Autoencoder is a popular machine learning model used for dimensionality reduction. Recently, it has become an important tool in generative AI. Recently, we have proposed autoencoder-with-ordered-variance as a tool to not just reduce the data dimensionality, but to also extract nonlinear models relating process variables. The resulting models can then be used for a variety of control, optimization, and monitoring related activities. This project will develop the ideas further both in terms of theoretical aspects as well as deploy the approach for high dimensional systems using deep learning and use the resulting model for process control and optimization activities. One of our recent work is available at: https://arxiv.org/abs/2402.14031	Control and Automation	Theoretical / Computational / Modelling	
	TA-AC	nagappan@iitb.ac.in	Nagappan Ramaswamy	Proton Exchange Membrane Water Electrolyzer Development for Hydrogen Generation	1) Proton exchange membrane water electrolyzers (PEMWE) are at the forefront of commercialization for green hydrogen generation 2) The energy conversion efficiency and the cost of hydrogen generated needs to be decreased to enable commercial success 3) The cost of PEMWE is high due to the use of precious iridium based electrocatalysts and thick perfluorosulfonic acid (PFSA) membrane electrolytes 4) This project will focus on redesigning PEMWE stack by decreasing the amount of iridium electrocatalyst by one of magnitude and decreasing the thickness of PFSA electrolyte by five-fold. 5) Understand the pros and cons of the new PEMWE design and develop areas for successful commercialization.	Water electrolyzers	Experimental	Chemical Engg, Chemistry, Materials Science or related field.

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	TA-AD	nagappan@iitb.ac.in	Nagappan Ramaswamy	Alkaline water electrolyzer	1) Alkaline water electrolyzer (AWE) technology enables lower cost of hydrogen generated due to inherently lower cost due to the use of inexpensive catalysts and electrolytes 2) However, AWE face major challenges due to low pressure operation, corrosion due to highly concentrated caustic electrolytes, low temperature operation, poor electrode stability under dynamic operation and low current density operation. 3) This project will identify the major reasons for these limitations and address them from the perspective of the electrolyzer components. 4) Develop electrocatalyst and electrochemical cell designs to address these challenges. 5) Develop Alkaline Anion Exchange Membrane Water Electrolyzer to mitigate some of these challenges via high pressure operation and improved electrode stability.	Alkaline water electrolyzer	Experimental	Chemical Engineering, Chemistry, Materials Science
	TA-AE	nagappan@iitb.ac.in	Nagappan Ramaswamy	Durable Fuel Cell Electrode Design for Electric Vehicle Applications	1) Proton exchange membrane (PEM) fuel cells are an alternative technology for clean, zero-emission automotive electric vehicles. They are expensive due to the use of precious platinum based electrocatalysts in the fuel cells. 2) Further, the durability of the platinum based fuel cell electrocatalysts need to be improved to decrease the total cost of ownership of the electric vehicles. 3) This project will focus on various strategies to develop durable fuel cell electrodes using strategies such as i) corrosion resistant catalyst development and ii) efficient distribution of the ionomer. 4) The project will focus on catalyst material development, electrode fabrication and fuel cell operation using various durability protocols.	Fuel cell electric vehicles	Experimental	Chemical engineering, chemistry or materials science
	TA-AF	nagappan@iitb.ac.in	Nagappan Ramaswamy	Electrocatalyst design for durable fuel cell electric vehicle applications	1) This project will focus on synthesizing novel electrocatalyst structure for durable fuel cell operation 2) Novel catalyst designs involve the shell-protected and in-pore structures. 3) Shell-protected catalyst structures involve designing carbon or metal oxide structure on platinum based catalysts 4) In-pore catalyst designs involve the use of porous carbon supports and developing strategies to deposit platinum nanoparticle catalysts predominantly inside the porous structure to improve performance durability 5) This project will focus on catalyst synthesis techniques and fuel cell operation.	Fuel cell electric vehicles	Experimental	Chemical engineering, chemistry, materials science
	TA-AG	p.sunthar@iitb.ac.in	P Sunthar	Optimizing Lithium-Ion Battery Cycles for Maximised Lifetime and Safety	The performance and lifespan of Lithium Ion Batteries (LIBs are limited by the irreversible degradation in a battery cell. This project aims to understand the processes at the cell level to obtain optimal charging and discharging protocols for various load demands and renewable energy production rates. We will employ tools such as Discrete Element Method (DEM) and physics-assisted machine learning (PAML) and physics-informed neural networks (PINN) in an attempt to solve the problem. https://www.che.iitb.ac.in/phd-ta-topic/optimizing-lithium-ion-battery-cycles-maximised-lifetime-and-safety	Modelling	Theoretical / Computational / Modelling	Chemical engineering, Physics, Python programming
	TA-AH	dasgupta.ratul@iitb.ac.in	Ratul Dasgupta	DNS & LES of surface and internal gravity waves - critical layer induced instabilities and their role in wave breaking	This is a jointly supervised project with Prof. Ravichandran at Climate Studies (IITB). The student will investigate surface and internal gravity waves in the ocean and how critical layer (where flow speed equals a wave speed and accompanying curvature in the shear flow profile) can trigger instabilities eventually leading to surface and internal wave breaking. Wave breaking both at the surface and in the deep ocean has strong consequences for long term climate models.	Fluid Mechanics	Theoretical / Computational / Modelling	Chemical / Mechanical / Aerospace/ Physics
	TA-AI	dasgupta.ratul@iitb.ac.in	Ratul Dasgupta	Wave-ice interaction : Theory and DNS	The project will conduct theory & DNS of wave ice interaction with an aim towards understanding how surface waves and icesheets interact with each other in the ocean. Such studies are becoming more and more important in the context of climate change. The work will be co-guided with Prof. Vatsal Sanjay (Assistant Professor, Physics Dept., Univ. Durham, United Kingdom - group to commence from July 2025,).	Fluid Mechanics	Theoretical / Computational / Modelling	Chemical / Mechanical / Aerospace / Physics
	TA-AJ	rochish@che.iitb.ac.in	Rochish M Thaokar	Experiments and phenomenonlogical as well as physics informed ML modeling of biomemetic excitable and unexcitable cells (GUVs)	Our group works on unexcitable and excitable biomemetic cells, made up of Giant Unilamellar Vesicles using experiments, theory and simulation as well. TThe objective in these works is to understand the complex multiphysics in these systems involving hydrodynamics, electrostatics and kinetics and membrane mechanics. In the past, we have conducted studies on electroporation and excitation of these systems. The proposed work will extend these studies for relevance to realising bio-memetic cells suitable for electroporation physics as well as extending phenomenological models to physics informed ML models. The work will involve all three components, experiments, theory and simulations. Recent references: Compound giant unilamellar vesicles as a bio-mimetic model for electrohydrodynamics of a nucleate cell R Kumar, R Chakrabarti, RM Thaokar Soft Matter 20 (35), 6995-7011, 2024 Electrohydrodynamics of vesicles and capsules K Priti Sinha, S Das, RB Karyappa, RM Thaokar, Langmuir 36 (18), 4863-4886, 2020	Biophysics	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering, Physics, Biotechnology,
	TA-AK	rochish@che.iitb.ac.in	Rochish M Thaokar	Novel electric field based physics for inventing novel sustainable processes for chemical industries and intensifying existing unit operations	Our group has been working on intensifying existing unit operations such as electrodesalters in oil refineries, and inventing new electric field based processes such as in indoor air cleaners. The approach is to understand and invent novel electric field based physics through hydrodynamic and chemical effects, and then employ then to devise new sustainable unit operations. The PhD will involve further progressing our research in electrodesalters and air cleaners but also explore newer unit operations, by conducting research in the fundamentals of electrohydrodynamics. The work will involve all three components, experiments, theory and simulations. Recent references: Electrocoalescence of a pair of conducting drops in an insulating oil, V Anand, S Roy, VM Naik, VA Juvekar, RM Thaokar, Journal of Fluid Mechanics 859, 839-850, 2019 Mitigating noncoalescence and chain formation in an electrocoalescer by electric field modulation, R Hasib, V Anand, VM Naik, VA Juvekar, RM Thaokar, Industrial & Engineering Chemistry Research 61 (46), 17145-17155, 2022	Process Intensification	Both: Theoretical (Computational or Modelling) + Experimental	Physics, Mechanical, Chemical
	TA-AL	srjadhav@iitb.ac.in	Sameer Jadhav	Dissipative Particle Dynamics simulation of peptide aggregation in phospholipid membranes	Dissipative particle dynamics (DPD) is a coarse-grained / mesoscopic simulation technique that allows simulation of larger systems with a limitation of reduced spatial and temporal resolution of events. We have previously used DPD to simulate phospho-lipid membranes and peptides separately. The goal of the present study is to simulate peptide aggregation leading to pore formation in phospholipid bilayers. This is important in understanding mechanisms underlying pore forming toxins as well as liposomal drug delivery. This work is in collaboration with Prof. Rochish Thaokar.	coarse grained molecular dynamics	Theoretical / Computational / Modelling	Chemical Engineering, Mechanical Engineering
	TA-AM	srjadhav@iitb.ac.in	Sameer Jadhav	Design, analysis and control of flow in microfluidic networks	Microfluidics technology has been seen to have great potential in lab-on-a-chip applications including chemical analysis and diagnostics. One may be able to control flow direction and flow rate as well as concentration of solutes in specific branches of the microfluidic network for certain designs of the network and the resistance to flow in each branch of the network. In this project we explore several designs and optimize geometric and flow parameters of the microfluidic network for desired flow and concentration patterns. The work is in collaboration with Prof. Ganesh Viswanathan.	Network Analysis	Theoretical / Computational / Modelling	B.Tech/M.Tech in Chemical Engineering, Mechanical Engineering or Biotechnology (with fluid mechanics subject).

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	TA-AN	sarika@che.iitb.ac.in	Sarika Mehra	Synthetic Biology tools to create host cell lines for production of recombinant proteins	A large number of therapeutics used to treat a range of diseases are recombinant proteins, that require mammalian cells as a host for their commercial production. Chinese hamster ovary (CHO) cell lines are the most preferred host cells for the production of a variety of biotherapeutics ranging from interferons to antibodies. Similarly, many vaccine candidates, such as the receptor binding domain of the SARS-COV2 are also produced in mammalian cells due to their glycosylation. The increasing demand to treat a variety of diseases has necessitated the need to increase the overall productivity of these therapeutic proteins. Further, the pandemic highlighted the need to shorten the clone development timelines for rapid production of antibodies and vaccine candidates. In this project, we will create a panel of cell lines based on genetic engineering targets identified in our lab and evaluate these cell lines for increased secretion of model recombinant proteins and Monoclonal Antibodies.	systems and synthetic biology	Experimental	Biotechnology/Molecular Biology/Chemical Engineering. Experience in cell culture or cloning will be a plus.
	TA-AO	sarika@che.iitb.ac.in	Sarika Mehra	Upstream Process development for recombinant therapeutics including MABs and vaccine subunits		biochemical engineering	Both: Theoretical (Computational or Modelling) + Experimental	Chemical Engineering/Biotechnology
	TA-AP	sonali.das@iitb.ac.in	Sonali Das	Catalyst development for applications in storage of green hydrogen in the form of liquid hydrogen carriers.	This project aims at the development of new catalysts and catalytic processes for the conversion of hydrogen into liquid hydrogen carriers and vice versa, which is an important step towards establishing a sustainable green hydrogen economy. The work would entail development of new catalyst materials, characterization, testing catalyst performance in reactors and detailed kinetic studies for green H2 applications.	Catalysis, Green Hydrogen, Sustainability	Experimental	
	TA-AQ	sonali.das@iitb.ac.in	Sonali Das	Catalyst and Process development for Plasma-catalytic Methane Valorization	This project aims at development of a lab-scale integrated plasma-catalytic reactor system incorporating novel catalysts for methane conversion to value-added higher hydrocarbons. Conversion of waste methane such as landfill gas etc. into value-added higher hydrocarbons is a highly desirable process in the context of environmental sustainability and greenhouse gas emissions. This project aims to use novel "plasma-catalysis" to accomplish this challenging conversion process. The work will entail development of new catalysts, characterization, catalyst testing. and design of plasma-catalytic hybrid reactors.	Catalysis, Nanomaterials, Sustainability	Experimental	
	TA-AR	sonali.das@iitb.ac.in	Sonali Das	Development of novel photothermal catalysts for sustainable carbon dioxide conversion using solar energy.	Converting CO2 into synthetic fuels and chemicals using sunlight as the sole energy source holds tremendous prospects for establishing a sustainable carbon-neutral economy. This project aims at developing novel photothermal catalysts to convert CO2 into value-added chemicals by harvesting both heating and optical properties of solar energy. The work will involve development of new nanomaterials (such as MOFs, core-shell catalysts), advanced material characterization, and photothermal reaction and reactor design.	Catalysis, nanomaterials, sustainability.	Experimental	
	TA-AS	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay	Machine Learning to Predict Stable Electrocatalysts Faster	When designing new materials, like next-generation batteries, catalysts, semiconductors, or systems for green hydrogen generation, researchers need to understand how atoms arrange themselves into stable configurations. This requirement is especially important in electrochemical reactions, such as those used in water splitting for hydrogen production, where the efficiency and stability of materials directly determine performance and cost. Finding these stable atomic structures is like solving a massive 3D puzzle with billions of possibilities. Traditionally, we've used physics-based search methods (like basin hopping or minima hopping) to explore the energy landscape of materials, hunting for the most stable configurations. While reliable, these methods are computationally expensive and slow, limiting the scale and speed at which we can create new materials. Now, there is an alternative approach: generative machine learning (ML). Instead of checking every possibility one-by-one, ML models learn from a database of known stable structures (generated using density functional theory, a simulation method). Architectures such as autoencoders, generative adversarial networks, and transformers can then generate new, stable structures much faster. What you will do in the project: (1) Develop state of the art machine learning methods from scratch (2) Compare traditional search methods with the machine learning models you develop (3) Perform large scale simulations on the fastest and most advanced high-performance computing clusters in India (4) Develop a nuanced understand of what types of problems machine learning is (or isn't) good at solving in chemical engineering Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group: https://www.che.iitb.ac.in/web/faculty/sv/	machine learning for science and engineering	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering or Chemistry and Physics who are curious about clean energy, catalysis, and computational modeling. You don't need prior experience in DFT or machine learning, just a willingness to learn.

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	TA-AT	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay	Understanding Catalyst Surfaces Using Quantum Mechanical and Analytical Models	This project focuses on using theory and computer simulations to understand how and why catalysts work, with the goal of designing better ones for important chemical and electrochemical reactions. We use theoretical models and simulations to study how molecules interact with the surfaces of catalysts. These surface interactions control how fast or efficiently a reaction occurs. For example, if molecules binds too weakly to the surface, the catalyst won't activate them. If they bind too strongly, the surface can get poisoned. The key is to find the right balance. We study these interactions using two main approaches: (1) Quantum mechanical simulations, such as density functional theory (DFT), which help us calculate how atoms and electrons behave on catalyst surfaces. Analytical models, like the Newns-Anderson model and related methods, which give us physical insight into how a material's electronic structure (such as the position of its d-band) affects reactivity. What you will do in this project: (1) Use density functional theory (DFT) to simulate how molecules bind and react on catalyst surfaces. (2) Learn and apply analytical models such as the Newns-Anderson model to understand how electronic structure controls catalytic activity. (3) Extend these models to include more realistic effects, such as electric fields, co-adsorption of molecules, and complex alloy surfaces. (4) Compare predictions from simple models with detailed quantum mechanical simulations to build physical intuition. (5) Identify trends and design principles that can help develop new catalysts for reactions like green hydrogen production and electrochemical energy conversion. By combining first-principles simulations with physics-based models, this project aims to develop a general theory of how surface chemistry works. This understanding can guide the design of new catalysts for processes like green hydrogen production, CO_2 reduction, or ammonia synthesis. Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group: https://www.che.iitb.ac.in/web/faculty/sv/	Catalysis	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering or Chemistry and Physics who are curious about clean energy, catalysis, and computational modeling. You don't need prior experience in DFT or machine learning, just a willingness to learn.
	TA-AU	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay	Bridging Atomistic Simulations and Machine Learning: Smarter Ways to Model Chemical Reactions	Understanding how atoms behave during chemical reactions is key to solving big challenges in fields like catalysis, energy storage, and electrochemistry. Traditionally, we use accurate but computationally expensive methods like density functional theory (DFT) to simulate these reactions. While powerful, DFT can only handle small systems and short time scales. To study real-world reactions, which happen over longer times and larger systems, we need faster tools. That's where machine learning models are particularly effective. By training machine-learned interatomic potentials (MLIPs) on atomic data, we can get DFT-level accuracy at a fraction of the cost. For these models to be reliable, they must be trained on the right kinds of atomic structures. This project explores smart ways to choose those structures, making the models both faster and more accurate. What you will do in this project: (1) Learn how machine learning models can predict atomic behavior in chemical reactions, using only a small amount of high-quality simulation data. (2) Explore two powerful selection strategies: Bayesian methods – to estimate the model's uncertainty and guide where more data is needed. Committee methods with neural networks – where a team of models "vote" on which data will help improve accuracy. (3) Apply and test these methods on example systems like metal oxides and water–ion mixtures that are relevant to real applications in electrocatalysis. You will run your calculations on fast computers in high performance computing clusters in India. Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group: https://www.che.iitb.ac.in/web/faculty/sv/	machine learning for science and engineering	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering or Chemistry and Physics who are curious about clean energy, catalysis, and computational modeling. You don't need prior experience in DFT or machine learning, just a willingness to learn.

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	TA-AV	sudarshan.vijay@iitb.ac.in	Sudarshan Vijay / Ojus Mohan	Designing Better Catalysts by Combining Industrial Data and Atomistic Simulations with Machine Learning	Chemical industries rely on catalysts to make reactions faster, more efficient, and more sustainable. However, designing new catalysts is often a slow, trial-and-error process. In this project, we're taking a new approach. We will combine industrial reactor data with atomic-level simulations to speed up catalyst design. We will use density functional theory (DFT). DFT is a type of quantum mechanical simulation tool that lets us predict how atoms and electrons behave in chemical systems. Using DFT, we can calculate how strongly molecules bind to a catalyst surface and what reaction barriers need to be overcome. While DFT gives us detailed information at the atomic level, it is limited in length and time-scale. On the other hand, industrial data (temperature, pressure, conversion, and selectivity) tells us how catalysts behave in full-scale reactors, but doesn't tell us what happening at the atomic level. Our goal is to connect these two pictures. We'll use generative machine learning models to learn patterns from both kinds of data and suggest new catalysts and optimal reaction conditions. What You Will Do in the Project: (1) Understand how DFT calculations are performed (2) Work with industrial reactor datasets to understand real-world catalytic performance (3) Train machine learning models that connect atomistic and industrial-scale data (4) Generate new catalyst ideas and reaction environments based on model predictions (5) Bridge fundamental science with real chemical engineering applications Why join the Theoretical Electrocatalysis Group? We are a small, relatively new group at IIT Bombay. You'll work closely with all members, including the PI, and there's plenty of room for your ideas to shape the direction of the project. Our group develops and collaborates with leading developers of density functional theory codes around the world. In addition to advancing science, you'll also contribute to writing high-quality production code that is integrated into widely used simulation tools and directly impacts thousands of research groups globally. Your work will help power real computational research in labs across the world. See here for additional details about the group: https://www.che.iitb.ac.in/web/faculty/sv/	generative machine learning	Theoretical / Computational / Modelling	This project is ideal for students from Chemical Engineering who are curious about heterogeneous catalysis and machine learning. You don't need prior experience in DFT or machine learning, just a willingness to learn.
	TA-AW	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-AX	saini@che.iitb.ac.in	Supreet Saini	From genes to genomics, and beyond.	Units of inheritance (or genes) were first proposed by Mendel in 1860s. However, the chemical basis of genes was not understood for another 100 years. This means that the definition and understanding of the word "gene" has undergone radical transitions. In the era of genomics, the relative role of a single gene is again being redefined and understood. In this project, we will study the transition from genes to genomics, and what does the future of evolutionary biology holds.	Evolutionary biology	Theoretical/Computational	Strong interest in evolutionary biology and history.
	TA-AY	saini@che.iitb.ac.in	Supreet Saini	Role of epistasis in dictating evolution of SARS CoV-2	SARS CoV-2 variants keep getting detected. However, does evolution of newer viral variants follow certain rules? How do the mutations that have already occurred and spread in populations dictate the future evolution of the virus? In this work, we will study the sequence evolution of SARS CoV-2 virus variants, and develop a framework to understand how epistasis constrains and/or facilitates evolution.	Evolution	Theoretical/Computational	Interest in Evolutionary Biology; Prior experience/comfort in coding.
	TA-AZ	swaticb@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.
	TA-BA	swaticb@iitb.ac.in	Swati Bhattacharya	Using computer simulations to find a cure for diabetes	As of 2025, approximately 9.6% of India's population aged 20 to 79 years is affected by diabetes, according to World Bank data. In absolute numbers, this translates to over 212 million people, making India the country with the highest number of individuals living with diabetes globally. The prevalence is higher in urban areas (11.2%) compared to rural areas (5.2%), and a significant portion of cases remain undiagnosed. Intrinsically disordered proteins (IDPs) are deeply involved in the pathogenesis of type 2 diabetes mellitus (T2DM) due to their flexible structures, which enable them to interact with multiple molecules and regulate key biological processes. Proteins such as IRS1, IRS2, and IRS4, which mediate insulin signaling, are highly disordered and play crucial roles in glucose metabolism. Their disordered regions often serve as hubs for protein-protein interactions and post-translational modifications, which are essential for proper insulin function. Dysregulation of these IDPs can impair signaling pathways, contributing to insulin resistance and hyperglycemia. Understanding the functional roles of IDPs in diabetes provides insights into novel therapeutic targets, potentially paving the way for innovative drug discovery aimed at stabilizing or modulating their activity. Using state-of-the-art computer simulations we will reveal structural details of IDPs involved in the pathogenesis of T2DM, identify temporary folds or binding sites, that might contribute to diabetes when disrupted. By understanding IDPs' dynamic behavior, researchers can design drugs that stabilize or block their harmful interactions—opening doors to treatments that were previously impossible to develop.	Computational Biophysics	Theoretical / Computational / Modelling	Students from chemical engineering, chemistry, physics, engineering physics, Biotech/BioEngineering.
	TA-BB	venkatg@iitb.ac.in	Venkat Gundabala	Development of nanomaterial-microparticle composites for sensing applications using microfluidics	Polymeric microparticles embedded with nanomaterials have applications in drug delivery, tissue engineering, biosensing, and catalysis. Existing conventional methods to synthesize these materials suffer from drawbacks such as complex fabrication, lack of control over size, non-uniform encapsulation/coating, etc. Microfluidics, with its superior control over process parameters, is an ideal alternative to existing fabrication techniques. In this project, the student will a) design and fabricate microfluidic devices for synthesis of nanomaterial-microparticle composites, b) optimize the process parameters for controlling the size, composition, and morphology of these composites, and c) test them for sensing applications. The project is predominantly experimental in nature. Reference Wang, W. E. I., Zhang, M. J., & Chu, L. Y. (2014). Functional polymeric microparticles engineered from controllable microfluidic emulsions. Accounts of chemical research, 47(2), 373-384.	Microfluidics	Experimental	Chemical engineering, Nanotechnology, Materials engineering, Experimental background

Department of Chemical Engineering, IIT Bombay.
List of TAP, FA, and TA Ph.D Topics for Autumn 2024-2025 (May 2025)
You have to submit your preferences based on the following topics on or before 26-Apr-2025 in the google form shared in the departmental (Chemical Engineering) website

	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-BC	venkatg@iitb.ac.in	Venkat Gundabala (Supervisor) and Mahesh Tirumkudulu (Co-supervisor)	Biodegradable Antibacterial Implant for Localised Prevention and Management of Bone Infections	Biodegradable antibacterial systems offer a promising localised drug delivery strategy for the prevention and management of osteomyelitis. Composed of biocompatible polymers or composites, these systems enable sustained, site-specific antibiotic release, maintaining therapeutic levels at the bone–tissue interface while minimising systemic toxicity. The architecture of the composite supports high drug loading and cellular infiltration, promoting both antimicrobial efficacy and tissue regeneration. Importantly, the combination of controlled antibiotic release and intrinsic antibacterial properties prevents bacterial adhesion and biofilm formation, mitigating colonisation at the implantation site. The complete biodegradation into non-toxic byproducts eliminates the need for surgical removal, presenting a clinically effective and patient friendly solution. In this project, the student will develop biodegradable implants for localised delivery of antibiotics to bone tissue, characterize their biodegradability, mechanical strength, release kinetics, and perform in vitro experiments to test their efficacy in preventing microbial growth. Reference Nie, B. E., Huo, S., Qu, X., Guo, J., Liu, X., Hong, Q., & Yue, B. (2022). Bone infection site targeting nanoparticle-antibiotics delivery vehicle to enhance treatment efficacy of orthopedic implant related infection. Bioactive Materials, 16, 134-148.	Healthcare	Experimental	Chemical engineering, Biotechnology, Experimental experience
	TA-BD	yshastri@iitb.ac.in	Yogendra Shastri	Sustainable Energy Transition Planning for India - Modeling and Analysis	India is on a path of rapid socio-economic transformation and has set ambitious targets to increase the size of its economy. India has also committed to achieve net zero status by 2070. To achieve this target, the energy sector has to lead the transition. This transition also needs to follow sustainability principles. The key objectives of this project are to address the following questions: - How can specific sectors, such as oil and gas, plan the transition for net-zero? - Which technologies are likely to succeed and must be prioritized (e.g., green hydrogen, biofuels, e-fuels etc.)? - What are the desirable and expected timelines for the adoption of these technologies? - How do the different transition pathways compare in terms of the sustainability? This is completely computational work, and is quite interdisciplinary.	Energy and sustainability	Theoretical / Computational / Modelling	Chemical Engineering