Department of Chemical Engineering, IIT Bombay.
Preference for TA, TAP and FA Ph.D Topics for Autumn, 2023-2024
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Topic No	Type of the project	Email Address of the faculty	Name of the faculty	Title of the project	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
1-TAP(Sbh)	TAP	bhartiya@che.iitb.ac.in	Sharad Bhartiya	Quasi-linear Parameter Varying Systems Representation and Control of Nonlinear Chemical Processes: A Machine Learning Approach	The primary objective is developing techniques to map LSTM or other RNNs to Q-LPV models as a control relevant, secondary digital twin and frozen parameter QLPV based fast MPC. The methods will be tested on single unit operation or a benchmark flowsheet level chemical process.	Model Predictive Control	Includes both, experiments and modeling	Chemical Engineering/ Systems and control/ Strong liking for coding in Matlab/Python
2-TAP(SS)	TAP	saini@che.iitb.ac.in	Supreet Saini	Investigation of metabolic cooperation driven evolutionary dynamics.	Species interact with each other via a number of ways. These include trade of metabolic products or intermediates. How this trade influences evolutionary trajectory of a community is not well understood. In this work, we will (a) design experiments using yeast and bacteria and (b) develop theory to investigate the role of metabolic trade in dictating evolutionary trajectories of species and communities.	Evolutionary Biology	Includes both, experiments and modeling	Strong interest in evolutionary biology.
3-TAP(OM)	TAP	ojus@iitb.ac.in	Ojus Mohan	Investigating CO2 conversion to methanol: A combined experimental and computational study	Converting CO_2 into value-added products offers the benefit of both reducing CO_2 emissions and generating useful chemicals. Methanol is a widely used industrial chemical and fuel, and its production from CO_2 can provide a sustainable and cost-effective alternative to conventional methanol production methods. The objective of this research is to synthesize and characterize different catalysts for CO_2 to methanol conversion and to investigate the reaction mechanism using computational simulations. The results of this research will contribute to the development of sustainable and cost-effective methods for methanol production from CO_2. The experimental part of the project will be co-supervised by Prof. Sanjay Mahajani.	Catalysis	Includes both, experiments and modeling	
4-TAP(YS)	TAP	yshastri@iitb.ac.in	Yogendra Shastri	Optimization of regional mapping of agricultural residue for energy and chemicals	Multiple applications of agricultural residue such as bio-power, ethanol, biogas, chemicals, and bioplastics are proposed. The economic and environmental feasibility of these options varies and depend on region specific factors such as local residue availability, scale, seasonality, regional energy demands and so on. In this project, we will develop an optimization model to identify optimal regional mapping between residue and end uses. Specific objectives are: - Selection of technologies for evaluation - Detailed economic and environmental impact assessment (e.g. carbon and water footprint, particular matter pollution) - Develop a large scale optimization model - Apply model to India at district level and provide optimal mapping. This information will be used to recommend region specific (district or state level) utilization options for residue.	Optimization and sustainability	Theoretical/Computational	Chemical engineering, Industrial engineering, Operations research, Biotechnology
5-TAP(YS)	TAP	yshastri@iitb.ac.in	Yogendra Shastri	Studies on the effect of pre-treatment options on compressed biogas (CBG) production from biomass	Pretreatment of agricultural residue is very important to improve yield of biomass in anaerobic digestion so that production of compressed biogas (CBG) becomes economically feasible. In this work, we will study different pre-treatment options and their effects on the biogas yield. Starting with information about different technologies available in literature, we will conduct experiments for selected pretreatment options with industry collaborators. Based on the data collected/generated, economic assessment and life cycle analysis will be done. This information will be used to develop a raking of options based on multiple criteria. This project is in collaboration with industry partner (Indian Oil Corporation Limited).	Biofuels	Includes both, experiments and modeling	Chemical engineering, biotechnology, environmental engineering
6-TAP(SD)	TAP	sonali.das@iitb.ac.in	Sonali Das (sonali.das@iitb.ac.in)	Catalyst and process development for Plasma-catalytic Conversion of Methane to C2 Hydrocarbons.	This project is through CoE-OGE, IIT Bombay with BPCL and GAIL as industrial partners. Methane is a greenhouse gas that is often flared in current industrial practice. In light of the current climate change issues and changing energy landscape, the direct one-step conversion of methane to higher hydrocarbons using renewable energy sources is a much sought after goal. Non-thermal plasma (NTP) has emerged as a promising route to drive methane conversion to C2+ hydrocarbons and H_2 at ambient temperature. NTP driven methane conversion offers advantages of one-step methane upgradation, use of renewable electricity as power source, and low-temperature operation, but is constrained by high energy requirement and poor selectivity towards target hydrocarbon products. The objective of this project is to develop a lab-scale integrated plasma-catalytic reactor system incorporating novel, efficient, and selective catalysts for methane conversion to C2 hydrocarbons. The work will involve the synthesis and characterization of novel catalysts to increase plasma-catalytic methane conversion and C2 selectivity, development of a lab-scale plasma-catalytic reactor, testing of developed catalysts, operating parameter optimization, and plant-wide process modeling and techno-economic analysis. The project will involve both experimental work in new material development (such as single atom catalysts), new integrated processes (DBD plasma-catalysis), and theoretical modeling and optimization using software such as Aspen HYSYS. For more details, visit: https://sites.google.com/view/das-lab [1]	Catalysis	Includes both, experiments and modeling	Chemical Engineering

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7-TAP(SD)	TAP	sonali.das@iitb.ac.in	Sonali Das (sonali.das@iitb.ac.in)	Development of Photothermal Catalysts for Sustainable Conversion of Carbon Dioxide	Converting CO2 into synthetic fuels and chemicals using sunlight as the sole energy source holds tremendous prospects for establishing a sustainable carbon-neutral economy. "Photothermal" catalysis is an emerging field that employs plasmonic materials to utilize both thermal and photochemical contributions of sunlight to drive catalytic reactions. By utilizing the full spectrum of sunlight (UV, visible, and IR spectra), photothermal catalysts can achieve several orders of magnitude higher yields than traditional photocatalysts. Development of effective catalysts, that can synergistically harvest light and photothermally convert CO2, is critical for the further development and implementation of this new technology. The proposed research aims at developing tailormade photothermal catalysts for light-driven CO2 hydrogenation to solar fuels with precisely engineered morphology (such as hierarchical core-shell/ yolk-shell structures) that can facilitate synergistic functions of light harvesting, photon-to-heat conversion, and CO2 activation. A primary focus would be to study the effect of catalyst morphology and to develop rigorous structure-property relations that can be used to develop catalysts with high solar-to-fuel conversion efficiency. The work will involve development of new nanomaterials (such as MOFs, core-shell catalysts), advanced material characterization, and photothermal reaction and reactor design. A collaboration with National University of Singapore and Tohoku University, Japan is foreseen. For more details, visit: https://sites.google.com/view/das-lab [2]	Catalysis	Experimental	Chemical Engineering
8-TAP(JA)	TAP	adhikari@iitb.ac.in	Jhumpa Adhikari	Molecular Simulation & Experimental Studies on High-Value Bio-chemicals derived from Biomass Valorization	This project is in collaboration with IOC via Centre of Excellence in Oil, Gas & Energy, IIT Bombay. Fossil fuel derived chemicals are considered to be negatively impacting the environment. Lignocellulosic biomass is a promising alternative to fossil fuels as a raw material for the production of fuels and chemicals. In this project, we will use molecular simulation techniques (both MD and MC via open source software packages such as LAMMPS, GROMACS MCCCS Towhee and in-house codes), which are a cost effective tool to study phenomena such as phase equilibria of the individual components as well as their mixtures, and also to understand and gain insights into the molecular-level origins of the observable macroscopic properties. Experiments will be performed in conjunction with the molecular simulations, and the organic product stream and purified products will be characterized by utilizing state-of-the-art analytical techniques at IOC R & D. [3]	Renewable resources	Includes both, experiments and modeling	Interest in coding or learning to code; and performing experiments
9-TAP(JA)	TAP	adhikari@iitb.ac.in	Jhumpa Adhikari	Understanding the Solution Thermodynamics of Natural Products Separation via Molecular Simulation Techniques	This project involves development of computational scheme for molecular simulation based rational solvent design for separation of natural products. This study is necessary as natural products find applications or have potential applications in diverse fields including drug discovery, biosynthesis, development of functional nanomaterials, etc.; though a small yield of natural products requires collection and processing of large amounts of raw materials. Experimental studies, thus, may be time-consuming and expensive. Computational schemes are a suitable alternative which allow one to gain an understanding of the solution thermodynamics involved and based on this understanding identify/design efficient and novel solvents for extraction of natural products. Project will involve use of open source packages for MD and MC such as LAMMPS, GROMACS, NAMD, MCCCS Towhee and in-house codes. Simple experiments to study efficiency of identified/designed solvents also planned.	Molecular Simulation Based Rational Solvent Design	Theoretical/Computational	Interest in coding or learning to code
10-TAP(RT)	TAP	rochish@che.iitb.ac.in	Rochish M Thaokar	Experimental investigations in electrospray based filter less air cleaner	The use of charged droplets to treat pollutants and combustion products has been described in the literature since 1940s. It overcomes the problem of high pressure-drop in filtration and ozone generation in electric based air purification systems. The project aims at both, developing a fundamental understanding of interaction between charged droplets and aerosol particles and based on this learning building a prototype electrospray based air cleaner. The project would essentially involve conducting a series of experiments on understanding the fundamentals of droplet-particle interaction, using an in-house levitation device , namely the electrodynamic quadrupolar trap. Charged droplets and aerosols interact via hydrodynamic as well as electrostatic interaction. These understandings will be used to develop a scaled-up electrospray air cleaner. The essentials will involve developing a well formed electrospray, particle injection system, using instruments to quantify particle capture amongst others.	Electrohydodynamics, fluid mechanics	Experimental	Chemical Engineering

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11-TAP(AbM)	TAP	abhijitm@iitb.ac.in	Abhijit Majumder	To fabricate and validate Brain Tumor on Chip models for screening and testing of personalised cancer drugs	"Understanding tumor growth on dish has always been a challenge for its complex nature. It involves cell to cell contact between multiple cell types, complex tissue 3D architecture, tissue rigidity, designing nearby blood vessels etc. In the proposed work, we plan to develop ""Tumor on Chip." The project will have multiple parts such as developing blood vessels on chip, developing tumor micro-environment, and then finally assembling all the parts together. The model developed will help us in testing drugs for their ability to cross blood-brain barrier (https://en.wikipedia.org/wiki/Blood%E2%80%93brain_barrier). The work will involve microfluidics, micro-fabrication, and cell culture. " This work will be guided in collaboration with Prof. Debjani Paul, BSBE	Microlfuidics, Drug testing, organ on chip	Experimental	Chemical Engineer with interest in biology
12-TAP(AbM)	TAP	abhijitm@iitb.ac.in	Abhijit Majumder	To Study the Role of Mechanics in the Cancer Metastasis	1. To prepare and characterise materials with different viscoelasticity. 2. To understand the effect of viscoelasticity of the tumor microenvironment on breast cancer cells and their migration. 3. To model the observation obtained in objective 2. Check this for more details: https://www.sciencedirect.com/science/article/pii/S1742706121005729 This project will be co-supervised with Prof. Jyoti Seth, ChE [4]	Mechanobiology, Rheology, Cell Biology, Cancer	Includes both, experiments and modeling	Chemical Engineering with a knack for bio research/innovation or vice versa
13-TAP(PW)	TAP	wangikar@iitb.ac.in	Pramod Wangikar	Metabolomics-based identification of novel biomarkers for early diagnosis of chronic kidney disease	Chronic kidney disease (CKD), characterized by progressive loss of kidney function, is a major global health issue, especially among diabetes patients. Advanced CKD is associated with an increased risk of cardiovascular complications, and may necessitate hemodialysis or renal transplantation. However, current diagnostic tests employed for CKD, i.e. serum creatinine and urine albumin measurement, are prone to variability and error. In addition, they do not provide a definitive diagnosis and classification of the initial asymptomatic stages of CKD. Metabolomics analysis can highlight alterations in metabolite levels associated with disease onset and progression, and can be used to identify biomarkers that would be indicative of early stage CKD. The work would involve the LCMS and GCMS analysis of metabolites from blood plasma and urine samples of patients, followed by statistical analysis to identify and validate potential biomarkers for CKD. These biomarkers would be further correlated with biochemical pathways and known clinical and demographic factors with the goal of understanding disease mechanisms and developing a sensitive and accurate diagnostic test for CKD. The project is in collaboration with Dr. Rakesh Sahay (Professor & Head, Department of Endocrinology, Osmania Medical College & Osmania General Hospital, Hyderabad) and Dr Manisha Sahay (Professor and Head, Department of Nephrology, Osmania Medical College & Osmania General Hospital, Hyderabad).	Metabolomics, LCMS, GCMS	Experimental	Biochemistry, Biotechnology, life sciences. FA holders will also be considered.
14-TAP(SwB)	TAP	swaticb@iitb.ac.in	Swati Bhattacharya	Molecular Simulations of HIV-2 protein VpX	Our research group is primarily engaged in the investigation of protein dynamics and mechanisms with applications to intrinsic immunity and viral response, HIV therapeutics and enzymatic catalysis. The Ph.D project involves research into a retroviral protein called VpX that enables immunodeficiency retroviruses such as HIV-2 to counteract the host cell defences. The project involves using molecular dynamics simulations to get a mechanistic understanding of the interaction between the mammalian protein SAMHD1 and the retroviral protein VpX which could pave the way for the development of a new generation of anti-HIV drugs. The student will learn state of the art molecular simulations techniques and a variety of data-mining techniques that will enable them to process the trajectories.	Biomolecular SImulations	Theoretical/Computational	Chemical Engg/Chemistry/Physics . Knowledge and interest in coding is desirable.
15-TAP(JS)		jyotiseth@iitb.ac.in	Jyoti R. Seth	On-demand Jet Propulsion Fuel with High Solid Loading	A jet propulsion fuel containing suspended oxidizable nanoparticles has enhanced energy density than regular fuels. This is because the maximum calorific value of conventional jet propulsion (JP) fuels cane be as high as 36,000 MJ/m3. Addition of oxidisable nano particles with a calorific value of 136,000 MJ/m3 can yield multi-fold increase in the energy release per unit volume of fuel. However, creating stable suspensions of nanoparticles in the organic JP fuel medium is challenging as the particles quickly aggregate and settle causing failure in the propulsion system. Our lab has developed a novel method for (patent pending) for creating stable gelled propellant fuel. These suspensions are solid like at rest but flow freely as liquids under small applied pressures. The viscoelastic properties of the suspension are designed for easy use as an "on-demand" propellant fuel and with increased flight performance of the propulsion vehicles. This PhD project is aimed at developing an understanding of the rheological properties, flow behaviour and combustion properties of these fuels while implementing a process based on the lab scale protocol for bulk manufacturing of the gelled propellants, for their ultimate utilisation in a combustion set-up.	High energy density fuels	Includes both, experiments and modeling	Chemical Engineering, Chemistry, Physics

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16-TA(JP)	TA	picardo@iitb.ac.in	Jason Picardo	Visco-elastic CFD: turbulence at zero Reynolds number	This project will involve using (and extending) an in-house CFD code to simulate the turbulent flow of polymer solutions. We will focus on situations that correspond to intriguing and unexplained experimental observations, especially with regard to elastic turbulence at vanishing Re, which may be applied to improve mixing in microchannels and enhance underground oil-recovery. The student will gain experience in code development, in addition to expertise in Non-Newtonian fluid dynamics, and turbulence. For more info on the project: https://www.che.iitb.ac.in/index.php/phd-ta-topic/visco-elastic-cfd-turbulence-zero-reynolds-number Personal and group webpages: https://www.che.iitb.ac.in/faculty/jason-r-picardo https://www.che.iitb.ac.in/group/multiscale-fluid-dynamics	Computational fluid dynamics	Theoretical/Computational	The project relies heavily on fluid dynamics, math related to PDEs, and numerical methods, and will involve coding in Fortran and Python. A good background in these areas will be very useful; if you don't have a background in some of these areas then you must have a strong interest to learn them.
17-TA(JP)	TA	picardo@iitb.ac.in	Jason Picardo	Pattern formation amid turbulence: how large-scale order survives small-scale chaos	The vast majority of flows in our daily experience are turbulent and yet we see patterns all around us. Ordered arrays of cloud streets, (turbulent) wind-driven waves with distinct wavelengths, and---for a more exotic example---Jupiter's red spot all testify to the ability of ordered patterns to arise and persist amidst turbulent fluctuations. In this project, we will specifically focus on understanding how patterns with length and time scales much greater than the turbulent flow arise and survive. We will do this in the specific context of waves driven by a tangential flow of turbulent air over the surface of a liquid layer. As we gain insight into this problem, we will be able to address other situations as well, and thereby attempt to uncover some general principles underlying pattern formation in turbulent flows. For more info on the project: https://www.che.iitb.ac.in/index.php/phd-ta-topic/pattern-formation-amid-turbulence-how-large-scale-order-survives-small-scale-chaos Personal and group webpages: https://www.che.iitb.ac.in/faculty/jason-r-picardo https://www.che.iitb.ac.in/group/multiscale-fluid-dynamics	Pattern formation	Theoretical/Computational	This project will involve understanding and applying theories of pattern formation, stability analysis, and stochastic models of turbulence. Simulations will also be needed, but of simplified models, as the very nature of these problems precludes the use of direct numerical approaches. To get started, a knowledge of fluid dynamics, mathematics of ODEs and preferably also of PDEs is important. Experience using Matlab or Python is also useful. If you don't have a background in some of these areas, then don't worry---you can learn, but you must have a strong interest in them.
18-TA(SS)	TA	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.
19-TA(SS)	TA	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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20-TA(OM)	TA	ojus@iitb.ac.in	Ojus Mohan	Accelerating the Discovery of Bimetallic Catalysts for CO2 Conversion with DFT-assisted Machine Learning [5]	Machine learning can be a useful tool for predicting the activity and selectivity of bimetallic catalysts for CO2 conversion reactions. By training a machine learning model on a dataset of known catalysts and their performance in CO2 conversion reactions, the model can learn patterns and relationships between catalyst composition, structure, and reaction performance. The aim of this project is to develop a machine learning model for predicting the activity and selectivity of bimetallic catalysts for CO2 conversion reactions, with the assistance of density functional theory (DFT) calculations. The project will involve the collection and preparation of a dataset of bimetallic catalysts, DFT calculations to generate features that capture the electronic and geometric properties of the catalysts, the development and optimization of a machine learning model, and the use of the model to aid in the design of new bimetallic catalysts. This project will contribute to developing efficient and accurate screening methods for potential catalysts, leading to the discovery of novel, efficient, and selective bimetallic catalysts for CO2 conversion reactions. [6]	Catalysis	Theoretical/Computational	Knowledge in coding
21-TA(YS)	TA	yshastri@iitb.ac.in	Yogendra Shastri	Systems dynamics and optimization based design of sustainable transport sector in India	Decarbonization of the transport sector is important for India to achieve net zero status by 2070. A particular challenge for India is the rapid expansion of the personal vehicle segment in the next couple of decades. Multiple options such as electric vehicles (EVs), biofuels based vehicles, compressed biogas driven vehicles and so on are being promoted. The optimal adoption of these technologies should be a function of technology performance, cost, environmental impact and policies, all of which are a function of time. This project will extend the work we have done in developing a system dynamics modeling framework to study the adoption of various vehicle options and recommend strategies to promote a desired outcome for decarbonization. The framework needs to be extended further to make it more useful. Some of the key ideas include: - Considering the availability of resources for biofuels sector - Incorporating performance of vehicle with age and vehicle scrappage policy - Capturing diversity in consumer decision making through agent-based modeling (complex systems theory) - Modeling spatial uncertainty in the country in terms of infrastructure and environment impacts This project is completely computational. The nature of work is very interdisciplinary, going beyond the field of chemical engineering. The programming will be using MATLAB. Prior work can be found at: https://link.springer.com/article/10.1007/s10098-022-02398-8	Sustainability	Theoretical/Computational	Chemical engineering, industrial engineering, environmental engineering, operations research
22-TA(OM)	TA	ojus@iitb.ac.in	Ojus Mohan	Combined Experimental and Computational Investigation of Greenhouse Gas Adsorption on Biochar	Biochar, a carbon-rich product of the thermochemical conversion (such as pyrolysis) of biomass and organic waste, has been recognized as a scalable, carbon dioxide removal technology by the United Nations Intergovernmental Panel for Climate Change (IPCC). With its high surface area, biochar can adsorb a wide range of green house gas (GHG) molecules, and its properties, such as porosity and functional groups, can influence its ability to do so. However, the adsorption mechanism of GHGs on biochar is not fully understood. The aim of this project is to investigate the potential of biochar as a sorbent for greenhouse gases (GHGs). The project will involve a combination of experimental and computational techniques (quantum mechanical simulations) to study the adsorption behavior of GHGs on biochar. The experimental part of the project will be co-supervised by Prof. Anjali Jayakumar from Newcastle University and will be done with close collaboration with the UK Biochar Research Centre at University of Edinburgh. [7]	Adsorption	Includes both, experiments and modeling	
23-TA(BKS)	TA	bharat.k.suthar@gmail.com	Bhartkumar Suthar	Modeling and Simulation of Li-ion and Na-ion Batteries	This project relates to modeling and simulation of Li-ion and Na-ion batteries. Significant research is underway to improve the performance and life of battery technologies. These approaches includes innovation in varioius aspects such as battery design, electrode design (3-D electrodes), active material properties, electrolyte parameters, additives, heat dissipation strategeis, smart charging methodologies, pack design, smart decision making at the pack level etc. In order to rationally approach the above mentioned aspects, mathematical modeling and simulation of batteries provides an indispensible tool. This project relates developing models suitable for addressing some of these innovations.	Li-ion Batteries	Includes both, experiments and modeling	Chemical Engg/Physics. Numerical (Matlab, Python) and symbolic computational software (Mathematica/Maple) knowledge is preferred.

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24-TA(JA)	TA	adhikari@iitb.ac.in	Jhumpa Adhikari	Understanding the Solution Thermodynamics of Natural Products Separation via Molecular Simulation Techniques	This project involves development of computational scheme for molecular simulation based rational solvent design for separation of natural products. This study is necessary as natural products find applications or have potential applications in diverse fields including drug discovery, biosynthesis, development of functional nanomaterials, etc.; though a small yield of natural products requires collection and processing of large amounts of raw materials. Experimental studies, thus, may be time-consuming and expensive. Computational schemes are a suitable alternative which allow one to gain an understanding of the solution thermodynamics involved and based on this understanding identify/design efficient and novel solvents for extraction of natural products. Project will involve use of open source packages for MD and MC such as LAMMPS, GROMACS, NAMD, MCCCS Towhee and in-house codes. Simple experiments to study efficiency of identified/designed solvents also planned. [8]	Molecular Simulation Based Rational Solvent Design	Theoretical/Computational	Interest in coding or learning to code
25-TA(BKS)	TA	bharat.k.suthar@iitb.ac.in	Bharatkumar Suthar	Estimation of available capacity ((State of Charge or SoC) and state of health (SoH) of a battery	The available capacity (also known as remaining capacity or state of charge or SoC) of a battery is very critical parameter for various applications. For fast charging and discharging applications (such as electric vehicles, drone applications, battery driven power tools), the accuracy of SoC estimation will allow for more efficient and safer use of batteries. Accurate estimation of such quantities also help make sure that the battery is operating under pre-defined safety window. First part of the project involves learning about battery models and simulating the charge discharge behaviour (voltage, current and temperature data). Substantial part of the project will be focused on estimation of SoC using the noisy data (voltage, current and temperatures) obtained either via high fidelity models or experiments. Softwares/platform: Matlab/Python topics such as state and parameter estimation, electrochemical reaction engineering, computational/ numerical methods will be helpful.	Battery	Includes both, experiments and modeling	Softwares/platform: Matlab/Python topics such as transport and reaction engineering, state and parameter estimation, electrochemical reaction engineering, computational/ numerical methods will be helpful.
26-TA(SuJ)	TA	jogwar@iitb.ac.in	Sujit Jogwar	Design and control aspects of heat exchanger networks	Heat exchanger networks (HENs) are facilitators of energy integration in chemical industry. We have recently developed a novel concept of energy flow redistribution to optimise operation of heat exchanger networks. This project involves extending these ideas to batch HENs as well as develop/modify HEN design methodologies in the context of energy flow redistribution.	Process Systems Engineering	Theoretical/Computational	Chemical engineering background is preferable. Experience with numerical simulations will be beneficial.
27-TA-VG	TA	venkatg@iitb.ac.in	Venkat Gundabala	Nanoparticle-encapsulated microfibers as vehicles for targeted drug delivery	Microfluidics provides a facile platform for generation of several biomaterials such as particles, capsules, microfibers, etc. The versatility of microfluidics based methods arises from the ability to control size, morphology, and composition of the generated entities. In this project the student will use microfluidic devices to generate drug and nanoparticle encapsulated microfibers for targeted drug delivery in pancreatic cancer. The encapsulated nanoparticles (iron oxide) will allow magnetic based controlled release of the drug to the targeted site. The project will involve designing and fabrication of microfluidic devices, generation of nanoparticle encapsulated microfibers, their characterization, in vitro drug delivery studies.Co-supervised by Prof. Rajdip Bandyopadhyaya.	Targeted drug delivery	Experimental	The student is expected to have good experimental skills with keen interest in exploring inter-disciplinary fields. Prior experience in microfluidics or biological projects is a plus, while not essential.
28-TA(VG)	TA	venkatg@iitb.ac.in	Venkat Gundabala	Microfluidics based generation of biomaterials for 3D tumor modelling	Breast cancer is the most common cancer in women in India and accounts for 14% of all cancers in women with high prevalence and mortality rate. However, one of the major hindrances in drug discovery as well as drug screening is unavailability of suitable model system to mimic true tumor microenvironment (TME). In this project, the student will design and fabricate microfluidics based devices to generate 3D particles and core-shell microcapsules to mimic TME. The focus will be on controlling the shape, size, and stiffness through suitable manipulation of the fluids, their flow rates, and device geometry. The generated entities will be used to carry out investigations into the growth of tumor cells when co-cultured with other cells. Significant part of the project will involve designing and working with microfluidic devices and understanding the fluid mechanics behind the generation of these 3D biomaterials. Co-supervised by Prof. Abhijit Majumder.	Microfluidics	Experimental	The student is expected to have good experimental skills with keen interest in the engineering and design aspects of the project. Prior experience with microfluidics is a plus, while not essential.

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29-TA(VG)	TA	venkatg@iitb.ac.in	Venkat Gundabala	Development of Dual Drug Delivery Systems Using Microfluidics	In this project, the student will develop a droplet-based microfluidic approach to generation of double emulsion droplets that carry lipid nanoparticles (LNP) to be used as dual drug (hydrophilic and hydrophobic) delivering vehicles. 3D glass-PDMS hybrid microfluidic device fabricated in-house will be used for this purpose. The encapsulated liposome nanoparticles of the generated Dual Drug Delivery System (DDDS) will be characterized using fluorescence based imaging and high resolution synchrotron based small angle x-ray scattering (SAXS) techniques. The in-situ measurements will unravel the self-assembly mechanism during the formation of the nanoparticle-lipid complexes for improved structural stability. Using the newly designed microfluidic platform the student will test the loading, drug release and efficacy measurements of hydrophilic and hydrophobic drugs loaded into the LNP carrying double emulsions, for specific disease treatment. The proposed approach is expected to provide a facile, continuous, and cost-effective route to efficient delivery of both hydrophobic and hydrophilic drugs, hitherto a challenging proposition.	Dual Drug Delivery	Experimental	The student is expected to have good experimental skills with keen interest in exploring inter-disciplinary fields. Prior experience in microfluidics or biological projects is a plus, while not essential.
30-TA(AbM)	TA	abhijitm@iitb.ac.in	Abhijit Majumder (abhijitm@iitb.ac.in)	To fabricate and validate high-throughput microfludic device for screening and testing of personalised cancer drugs	Efficacy of chemotherapeutic drugs are often patient specific. The drug combination that works for one patient does not work well for other. In this project we aim to develop a microfluidic system that can be used to test the efficacy of a drug regime on patient specific biopsy samples.	Microlfuidics, Drug testing, organ on chip	Includes both, experiments and modeling	Chemical Engineering with a knack for bio research/innovation
31-TA(MV)	TA	madhu@che.iitb.ac.in	Madhu Vinjamur	Enhanced Diffusion-based Loading of Drugs on Mesoporous Silica from Supercritical Carbon dioxide	The use of mesoporous nanoparticles (MSPs) as carriers for drug delivery systems has gained importance, as they are now recognized as GRAS (Generally Recognized as Safe) for human intake. MSPs have a porous structure varying from 2-50 nm. These pores provide a high surface area for adsorption of drug, yielding high loadings due to their high surface area to volume ratios. However diffusional resistance of the solid drug to the pore surface often poses a problem. Recently DiSupLo (Diffusion Supported Loading) method using ethanol vapors was reported for fast, uniform and controlled drug loading on MSPs. However, at the end of the process ethanol requires removal from the solid mixture of the drug and MSPs through drying, which may clog the pores hindering release of the loaded drug from the pores. Moreover, ethanol may not be a suitable solvent for the drug. On the contrary, Supercritical carbon dioxide (scCO2) is known to solubilize a wide variety of drugs. It is GRAS and a green substitute to the traditional organic solvents. Moreover, removal of scCO2 at the end of the operation simply requires depressurization of the vessel. The present work will explore a new method: "Supercritically Enhanced Diffusion-based Loading" on MSPs by replacing ethanol with scCO2 for carrying the drug to MSP as the two would be uniformly homogenized as a solid mixture. There would be several advantages of the process, as diffusional resistance of the drug transfer to the bed heights of the porous MSPs would be minimized enabling uniform, fast, and efficient loading, thereby less amount of drug would be needed for making the drug formulation with MSPs of the desired loading having uniform concentration.	Drug delivery	Includes both, experiments and modeling	Chemical Engineering

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32-TA(MV)	TA	madhu@che.iitb.ac.in	Madhu Vinjamur	Drug Delivery using Supercritical Carbon Dioxide-Assisted Impregnation of Biocompatible Polymeric Implants	In recent years controlled drug delivery using various biodegradable or biocompatible polymeric implants has generated increasing interests by impregnating the desired therapeutic agents for sustaining the drug effect for a prolong time. Supercritical CO_2 –assisted impregnation of a drug, a protein or a vaccine on a polymeric carrier obviates the drawbacks of the conventional processes, such as, solubility and recrystallization. SC CO_2 can penetrate and plasticize the polymeric matrix, thereby creating a path way for the transport of the large molecules with structural stability and thus tailoring the morphology of the carrier for impregnation of the SC CO_2 soluble bioactive compounds. In this process, the drug is first solubilized in SC-CO_2 and then CO_2 plus drug is allowed to contact the polymer for impregnation of the drug. Various parameters such as solubility of the drug in SCCO2, absorption of SCCO2 into the polymer, and affinity between drug and polymer can influence the drug loading process and may affect the properties of the drug loaded implant. Numerous APIs (drugs, genes, or proteins) have been reported to be packed into various biocompatible polymeric implants (e.g.,PLA, PLGA, PCL, poly(methyl methacrylate) (PMMA), and others), biodegradable polymers (e.g., chitosan derivatives, and silicone-based copolymers) These implants have considerable mechanical strengths and have been envisioned for various biomedical applications, such as, ophthalmic, orthopedic stents, and other implantable medical devices to increase the bioavailability of the drugs. The present project aims to investigate SC CO_2 –assisted impregnation of two such polymers with pure and mixed drugs, analytically characterize them, and analyze the effects of operating pressure, temperature, drug concentration, depressurization rate, and the nature of the drug – polymer-CO_2 interactions on the loading and dissolution of the drugs from the SC CO_2 processed polymeric matrix, both experimentally and by mathematical modeling.	Drug delivery	Includes both, experiments and modeling	Chemical engineering
33-TA(AMS)	TA	amol.subhedar@iitb.ac.in	Amol Subhedar	A lattice Boltzmann model for three-phase flows	Three-phase flows are important for many industrial processes, such as enhanced oil recovery and membrane fuel cells. Accurate modeling of the three-phase flows essentially boils down to the correct treatment of the triple junction. To this end, we propose a velocity-based equilibrium distribution model in one class of the lattice Boltzmann method. The model will be analyzed in the sharp interface limit, and it will be applied to formation of droplets inside microfluidic devices.	fluid dynamics	Theoretical/Computational	
34-TA(GAV)	TA	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. [9]
35-TA(PSG)	TA	psg@iitb.ac.in	Partha S Goswami (psg@iitb.ac.in)	Effect of electrostatic force on the dynamics of particles in wall bounded channel flow: A DNS study.	The objective of this project is to understand the effect of electrostatic forces on small particles in a particle laden turbulent channel flow. An in-house direct numerical simulation (DNS) code is to be modified for this study. A detailed understanding of particle dynamics, their dispersion behavior and turbulence modulation will help towards the design of electrostatic precipitators. Student should have inclination towards CFD and theoretical fluid dynamics.	Multiphase flow CFD	Theoretical/Computational	Chemical Engg/Mechanical Engg/ Physics
36-TA(GAV)	TA	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.

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37-TA(PSG)	TA	psg@iitb.ac.in	Partha S. Goswami	Investigation of the particle (tablet) coating process in a spouted/fluidised or rotating bed using CFD-DEM approach	The present study aims to understand the tablet coating process by analyzing the residence time of the particles in the spray zone and the interaction between the droplets and the particles inside a spouted bed. Different models which describe particle motion, fluid-particle, and droplet-particle interactions will be integrated into open-source CDF software OpenFoam to achieve the above objective. Results will be compared with experimental data. For details refer to the following links: https://drive.google.com/file/d/1P2H-ZikU9ULstT5yEaPQOZKs-bVhExcK/view?usp=sharing https://drive.google.com/file/d/1DWGeMpQdcWwM9KLc_O5cW6YhMy611lm6/view?usp=sharing	CFD of coating	Includes both, experiments and modeling	Chemical Engg/Mechanical Engg/Knowledge in coding
38-TA(SRJ)	TA	srjadhav@iitb.ac.in	Sameer Jadhav	Analysis of biochemical signaling network for periodic forcing in sperm flagella.	Sperm motility is critical to fertilization and reproduction in animals. There remain several gaps in the knowledge base about the signaling mechanisms that govern conversion of chemical energy to mechanical work leading to flagellar beating as well as sperm steering and homing. The goal of this study is to build biochemical networks from available literature and propose models that explain and predict sperm motility in response to chemo-attractive molecules. Prof. Ganesh Viswanathan will be the co-Supervisor on this project.	biomechanics, systems biology	Theoretical/Computational	Chemical Engineering/Biochemical Engineering
39-TA(SRJ)	TA	srjadhav@iitb.ac.in	Sameer Jadhav	Flow analysis and control in microfluidic networks	Microfluidics technology has been seen to have great potential in lab-on-a-chip applications including chemical analysis and diagnostics. However, flow control in these networks requires either a pneumatic or fluidic control layer over the microfluidic layer. Recent studies have shown that integrated flow control may be achieved by introducing capacitive elements or obstacles in the flow path so that system response becomes non-linear as required for flow switching. In this project we explore several designs and optimize geometric and flow parameters of the microfluidic network for desired flow control. We intend to use Ansys® and OpenFOAM® (open source CFD software) for this project.	microfluidics, CFD	Theoretical/Computational	Chemical Engineering, Mechanical Engineering
40-TA(RB)	TA	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 is funded by DST. Most of the work will be experimental, with some scope of modeling, depending on student's interest.	Water	Experimental	

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41-TA(RB)	TA	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.		Includes both, experiments and modeling	Chemical Engg., Mechanical Engg., Physics, Theoretical Chemistry
42-TA(RB)	TA	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Development of polymeric implant for nanoparticle mediated drug delivery in pancreatic cancer	Pancreatic cancer is one of the cancers having the lowest 5-year survival rate, because of its late diagnosis and availability of only a couple of known drugs with very moderate increase in patient's survival. Based on our earlier work, we have shown that, nanoparticle mediated delivery of existing drugs can enhance the cytotoxicity in cancer cells. Accordingly, we have developed subcutaneous and orthotopic in-vivo experiments in mouse, in collaboration with Advanced Cancer Teaching Research and Education Centre (ACTREC), Navi Mumbai. The aim of this project will be to further increase the efficacy of this process, by making 3D printed, polymer-based implants in order to mimic the interaction of nanoparticles with cancer cells in a controlled microfluidic environment. The resulting insight will elucidate the optimization of the nanoparticle-based drug delivery system. We have already developed and further improving a film- and a gel-based implants. Some background or experimental exposure in any of the following is better: polymeric materials or nanomaterials or microfluidics or drug delivery. Chemical Engineering principles like transport phenomena, reaction engineering and life-sciences oriented skills in cell cultures, drug loading, release, cell dynamics will be useful. The project is funded by WRCB, IIT Bombay and it will be a work leading to learning and expertise in interdisciplinary research areas in chemical engineering, material science and biotechnology. The work will be in a group of students involving others already working in related parts of this project. The work will be mostly experimental, with some scope of modeling based on student's interest.	Drug delivery	Experimental	
43-TA(HN)	TA	hnanavati@iitb.ac.in	Hemant Nanavati	Accurate Molecular Models for Real Polymers (TA/FA)	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 [10]	Theoretical/Computational	Chemical Engg/Chemistry/Physics /Materials Science/Polymers/Knowledge in coding

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44-TA(HN)	TA	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers (TA / FA)	In this project, the aim is to understand quantitatively the molecular elasticity of biopolymers with potential engineering applications. The first example is Spider Dragline Silk, which may be several times stronger than steel (after normalizing the density). The work involves experimental, computational and theoretical analyses of the molecular structure of the biopolymer system.	Biopolymer Physics	Includes both, experiments and modeling	Chemical Engg/Chemistry/Physics /Materials Science/Polymers/Knowledge in coding
45-TA(AC)	TA	abhijit@che.iitb.ac.in	Abhijit Chatterjee (abhijit@che.iitb.ac.in)	Novel catalyst for electrocatalytic CO2 reduction reaction [11]	According to the Paris climate accord signed in 2016 with the aim of substantially lowering the risks and impacts of climate change, the goal is to pursue technologies that can limit the rise in average global temperature to ~1.5 degree C above the pre-industrial levels by 2050. One of the important greenhouse gas emissions being targeted is carbon dioxide. Currently, production of commodities crucially linked to growth and development, such as cement, steel, plastic, ammonia and aluminum, are resulting in large CO2 emissions. A promising upcoming technology is to utilize the CO2 emitted by electrochemically converting it to more higher energy products like carbon monoxide, methane, formic acid, methanol, ethanol, ethylene, etc. From the process economics point of view, the production of formic acid, propanol, ethanol, ethylene, etc. is viewed favorably, whereas, production of carbon monoxide, coal, methane, etc., is not favorable. We shall study the carbon dioxide reduction reaction CO2RR steps in a membrane electrode assembly using novel electrocatalysts. The electrochemical process can benefit from high activity and higher selectivity towards economically favorable chemicals, and process intensification.	Reaction engineering and catalysis	Includes both, experiments and modeling	Chemical engineering, chemistry
46-TA(SwB)	TA	swaticb@iitb.ac.in	Swati Bhattacharya	Modeling and Simulations of Sorcin, an oncoprotein associated with multi drug resistant cancers.	Sorcin is a calcium binding oncoprotein expressed at high levels in several human tumors such as leukemia, gastric, breast and ovarian cancers. Sorcin is an essential oncoprotein, which activates and regulates mitosis and cytokinesis. In recent years, there is growing evidence for its role in multi-drug resistant cancers. Our goal is to uncover its working through molecular simulations, understand its role in MDR cancers and attempt to find a druggable way to toggle its activity. The project will involve the study of the protein through all atom molecular simulations and ab initio methods.	Biomolecular Simulations	Theoretical/Computational	Chemical Engg/Chemistry/Physics. Coding sills desirable
47-TA(MT)	TA	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
48-TA(MT)	TA	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
49-TA(SBN)	TA	noronha@iitb.ac.in	Santosh Noronha	Enzyme bioreactors	The objective is to design and implement catalytic bioreactors. Work elements will involve standardization of a catalytic system, characterization of kinetic and transport aspects, process optimization, and detection in real time.	Bioreactor	Includes both, experiments and modeling	Exposure to process reaction engineering and/or biocatalysis would be an advantage.

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50-TA(YS)	TA	yshastri@iitb.ac.in	Yogendra Shastri	Sustainability assessment of technologies for decarbonization of energy sector	The global oil and gas industry is currently faced with the challenge of sustainable energy transition, a key driver of which is the need for reducing GHG emissions – ideally to a net-zero status – a process broadly described as "decarbonization" in the literature. This will require adoption of technologies such as carbon capture and sequestration and use of green hydrogen. Selection of the appropriate technology will depend on the decarbonization potential, cost, scalability, and technology readiness level. The student working on this topic will study one or more of these ideas is details. The work will involve some of the following specific tasks: - Identify decarbonization technology options for renewable hydrogen and carbon capture and utilization/storage (CCU/CCS) - Perform sustainability assessment considering economic, environmental, safety, and social dimensions using tools such as LCA. - Provide recommendations based on LCA, TEA and technology readiness level - Assess the suitability of the recommendation for specific sectors such as oil and gas This work is completely computational in nature and may involve active interaction with experts from industries. Student working on this project will need to develop expertise in process design and modeling, mass and energy balance, and process integration. Additionally, the student will also need to learn life cycle assessment, techno-economic assessment, and mathematical optimization methods.	Energy sector decarbonization	Theoretical/Computational	Chemical engineering
51-TA(RaD)	TA	dasgupta.ratul@gmail.com	Ratul Dasgupta	Mass transport due to water waves	The aim of this project is to study a nonlinear process which causes mass transport in water waves. The first study of this was by George Gabriel Stokes (one of the two names in Navier-Stokes equations) who showed that when non-linear effects are (partly) accounted for, the trajectory of a fluid parcel due to a travelling surface wave is not closed and contains a small net displacement in the direction of wave propagation. Averaged over several thousand wave periods, this can causes substantial drift of particles in the direction of the wave propagation and plays an important role in the transport of sediments in the ocean. In the context of Faraday waves (standing waves first observed by Michael Faraday), similar drift patterns have been uncovered in the last twenty years and are referred to under the general label streaming. Streaming is not specific to water waves and occur in general wave systems. It is known in acoustic waves (inside the human ear for example) and in wall attached boundary layers. The aim of this project is to investigate streaming and mass transport in the context of travelling and standing water waves, with the goal of understanding how waves transport sand particles. The work will be mathematical and computational in nature. Please apply if you are fascinated by maths, physics and fluid dynamics. A background in CFD will help although not strictly necessary. If you are excited with doing theory, this is a very suitable project.	Fluid Mechanics and transport	Theoretical/Computational	Chemical Engg. , Mechanical Engg. , Aerospace Engg. or MSc Physics
52-TA(SBh)	TA	sharad_bhartiya@iitb.ac.in	Sharad Bhartiya, Vinay Juvekar Sanjay Mahajani [12]	A Sugarcane-based Biorefinery: Development of high value nutraceuticals using chromatographic methods	FIlter press mud is usually discarded or used as compost while bagasse is used for its fuel value. It is well known that these residues contain high-value micro and macro-nutrients. These include nutraceutical compounds such as policosanols (linear chain alcohols) that have been shown to possess health benefits in relation to Parkinson's treatment and cholesterol-lowering ability. In this work, we propose to develop continuous chromatographic methods to extract and purify octacosanol and other policosanols from press mud after the extraction step thereby enabling the filter press mud, a reject from the sugar industry to be monetized.	Separation processes	Includes both, experiments and modeling	Chemical Engineering, chemistry

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You have to submit your preferences based on the following topics on or before 04/05/2023 in the google form shared in the departmental (Chemical Engineering) website
You should attend the online discussion session to know "How to fill the preference form" on 29-Apr-2023

Topic No	Type of the project	Email Address of the faculty	Name of the faculty	Title of the project	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
53-TA(JS)	TA	jyotiseth@iitb.ac.in	Jyoti R. Seth	On-demand Jet Propulsion Fuel with High Solid Loading	A jet propulsion fuel containing suspended oxidizable nanoparticles has enhanced energy density than regular fuels. This is because the maximum calorific value of conventional jet propulsion (JP) fuels cane be as high as 36,000 MJ/m3. Addition of oxidisable nano particles with a calorific value of 136,000 MJ/m3 can yield multi-fold increase in the energy release per unit volume of fuel. However, creating stable suspensions of nanoparticles in the organic JP fuel medium is challenging as the particles quickly aggregate and settle causing failure in the propulsion system. Our lab has developed a novel method for (patent pending) for creating stable gelled propellant fuel. These suspensions are solid like at rest but flow freely as liquids under small applied pressures. The viscoelastic properties of the suspension are designed for easy use as an "on-demand" propellant fuel and with increased flight performance of the propulsion vehicles. This PhD project is aimed at developing an understanding of the rheological properties, flow behaviour and combustion properties of these fuels while implementing a process based on the lab scale protocol for bulk manufacturing of the gelled propellants, for their ultimate utilisation in a combustion set-up.	High Energy Density Fuels	Includes both, experiments and modeling	Chemical Engineering, Chemistry, Physics
54-TA(JS)	TA	jyotiseth@iitb.ac.in	Jyoti R. Seth	Three-dimensional Self Assembly of Graphene	Three-dimensional (3D) graphene is known to have numerous applications as adsorbent, catalysts, sensors, energy storage such as batteries and super-capacitors. Further, 3D graphene is easy to handle and convenient to load as adsorbent in a packed bed. One of the ways of preparing 3D graphene is through reduction of 2D graphene oxide particles which leads to self-assembly of the reduced graphene particles in to a 3D "house of cards" type structure. However, this resultant structure has to have mechanical strength as well as flexibility and compressibility so that it is amenable to be used as packing in large scale industrial columns. At the same time, the surface area of the original 2D graphene oxide must be preserved, to the extent possible, so that the properties of 2D graphene such as conductivity and surface area are conserved. The aim of this PhD topic would be to develop techniques for preparation of 3D graphene in order to achieve desired characteristics as mentioned above. Influence of methods of reduction, types of reducing agents, kinetics of reduction and various other parameters on the number as well as strength of connections between reduced graphene particles will be studied. The dynamics of the self-assembly will also be studied through an analogous experimental system involving 3D printed sheet-like particles representing graphene. Embedded magnets in the particles will be used to tune particle-particle attraction. This work is in collaboration with Dr. Per Loethman of Foviatech GmBH (https://www.foviatech.com). The selected student may spend some time at our collaborator's lab in Germany. A collaboration with University of Delft in Netherlands is also foreseen. Further information can be found on https://www.che.iitb.ac.in/phd-ta-topic/three-dimensional-self-assembly-graphene	3D Graphene	Includes both, experiments and modeling	Chemical Engineering, Chemistry, Physics
Only those candidates who have external fellowsip/s like CSIR/DBT JRF can opt for the following topis [55-FA(SS) to 72-FA(SMM)]								
55-FA(SS)	FA	saini@che.iitb.ac.in	Supreet Saini	Role of epistasis in dictating SARS CoV-2 evolution.	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 in coding.
56-FA(VG)	FA	venkatg@iitb.ac.in	Venkat Gundabala	Nanoparticle-encapsulated microfibers as vehicles for targeted drug delivery	Microfluidics provides a facile platform for generation of several biomaterials such as particles, capsules, microfibers, etc. The versatility of microfluidics based methods arises from the ability to control size, morphology, and composition of the generated entities. In this project the student will use microfluidic devices to generate drug and nanoparticle encapsulated microfibers for targeted drug delivery in pancreatic cancer. The encapsulated nanoparticles (iron oxide) will allow magnetic based controlled release of the drug to the targeted site. The project will involve designing and fabrication of microfluidic devices, generation of nanoparticle encapsulated microfibers, their characterization, in vitro drug delivery studies.Co-supervised by Prof. Rajdip Bandyopadhyaya.	Targeted drug delivery	Experimental	The student is expected to have good experimental skills with keen interest in exploring inter-disciplinary fields. Prior experience in microfluidics or biological projects is a plus, while not essential.

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57-FA(VG)	FA	venkatg@iitb.ac.in	Venkat Gundabala	Microfluidics based generation of biomaterials for 3D tumor modelling	Breast cancer is the most common cancer in women in India and accounts for 14% of all cancers in women with high prevalence and mortality rate. However, one of the major hindrances in drug discovery as well as drug screening is unavailability of suitable model system to mimic true tumor microenvironment (TME). In this project, the student will design and fabricate microfluidics based devices to generate 3D particles and core-shell microcapsules to mimic TME. The focus will be on controlling the shape, size, and stiffness through suitable manipulation of the fluids, their flow rates, and device geometry. The generated entities will be used to carry out investigations into the growth of tumor cells when co-cultured with other cells. Significant part of the project will involve designing and working with microfluidic devices and understanding the fluid mechanics behind the generation of these 3D biomaterials. Co-supervised by Prof. Abhijit Majumder.	Microfluidics	Experimental	The student is expected to have good experimental skills with keen interest in the engineering and design aspects of the project. Prior experience with microfluidics is a plus, while not essential.
58-FA(VG)	FA	venkatg@iitb.ac.in	Venkat Gundabala	Development of Dual Drug Delivery Systems Using Microfluidics	In this project, the student will develop a droplet-based microfluidic approach to generation of double emulsion droplets that carry lipid nanoparticles (LNP) to be used as dual drug (hydrophilic and hydrophobic) delivering vehicles. 3D glass-PDMS hybrid microfluidic device fabricated in-house will be used for this purpose. The encapsulated liposome nanoparticles of the generated Dual Drug Delivery System (DDDS) will be characterized using fluorescence based imaging and high resolution synchrotron based small angle x-ray scattering (SAXS) techniques. The in-situ measurements will unravel the self-assembly mechanism during the formation of the nanoparticle-lipid complexes for improved structural stability. Using the newly designed microfluidic platform the student will test the loading, drug release and efficacy measurements of hydrophilic and hydrophobic drugs loaded into the LNP carrying double emulsions, for specific disease treatment. The proposed approach is expected to provide a facile, continuous, and cost-effective route to efficient delivery of both hydrophobic and hydrophilic drugs, hitherto a challenging proposition.	Dual Drug Delivery	Experimental	The student is expected to have good experimental skills with keen interest in exploring inter-disciplinary fields. Prior experience in microfluidics or biological projects is a plus, while not essential.
59-FA(AbM)	FA	abhijitm@iitb.ac.in	Abhijit Majumder	To fabricate and validate high-throughput microfludic device for screening and testing of personalised cancer drugs	Efficacy of chemotherapeutic drugs are often patient specific. The drug combination that works for one patient does not work well for other. In this project we aim to develop a microfluidic system that can be used to test the efficacy of a drug regime on patient specific biopsy samples.	Microlfuidics, Drug testing, organ on chip	Experimental	Biotech with an interest in making devices/innovation
60-FA(GAV)	FA	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. [13]
61-FA(GAV)	FA	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.
62-FA(SRJ)	FA	srjadhav@iitb.ac.in	Sameer Jadhav	Analysis of biochemical signaling network for periodic forcing in sperm flagella.	Sperm motility is critical to fertilization and reproduction in animals. There remain several gaps in the knowledge base about the signaling mechanisms that govern conversion of chemical energy to mechanical work leading to flagellar beating as well as sperm steering and homing. The goal of this study is to build biochemical networks from available literature and propose models that explain and predict sperm motility in response to chemo-attractive molecules. Prof. Ganesh Viswanathan will be the co-Supervisor on this project.	biomechanics, systems biology	Theoretical/Computational	Chemical Engineering/Biochemical Engineering

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63-FA(RB)	FA	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 is funded by DST. Most of the work will be experimental, with some scope of modeling, depending on student's interest.	Water	Experimental	
64-FA(RB)	FA	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Development of polymeric implant for nanoparticle mediated drug delivery in pancreatic cancer	Pancreatic cancer is one of the cancers having the lowest 5-year survival rate, because of its late diagnosis and availability of only a couple of known drugs with very moderate increase in patient's survival. Based on our earlier work, we have shown that, nanoparticle mediated delivery of existing drugs can enhance the cytotoxicity in cancer cells. Accordingly, we have developed subcutaneous and orthotopic in-vivo experiments in mouse, in collaboration with Advanced Cancer Teaching Research and Education Centre (ACTREC), Navi Mumbai. The aim of this project will be to further increase the efficacy of this process, by making 3D printed, polymer-based implants in order to mimic the interaction of nanoparticles with cancer cells in a controlled microfluidic environment. The resulting insight will elucidate the optimization of the nanoparticle-based drug delivery system. We have already developed and further improving a film- and a gel-based implants. Some background or experimental exposure in any of the following is better: polymeric materials or nanomaterials or microfluidics or drug delivery. Chemical Engineering principles like transport phenomena, reaction engineering and life-sciences oriented skills in cell cultures, drug loading, release, cell dynamics will be useful. The project is funded by WRCB, IIT Bombay and it will be a work leading to learning and expertise in interdisciplinary research areas in chemical engineering, material science and biotechnology. The work will be in a group of students involving others already working in related parts of this project. The work will be mostly experimental, with some scope of modeling based on student's interest.	Drug delivery	Experimental	
65-FA(HN)	FA	hnanavati@iitb.ac.in	Hemant Nanavati	Accurate Molecular Models for Real Polymers (TA/FA)	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 [14]	Theoretical/Computational	Chemical Engg/Chemistry/Physics /Materials Science/Polymers/Knowledge in coding
66-FA(HN)	FA	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers (TA / FA)	In this project, the aim is to understand quantitatively the molecular elasticity of biopolymers with potential engineering applications. The first example is Spider Dragline Silk, which may be several times stronger than steel (after normalizing the density). The work involves experimental, computational and theoretical analyses of the molecular structure of the biopolymer system.	Biopolymer Physics	Includes both, experiments and modeling	Chemical Engg/Chemistry/Physics /Materials Science/Polymers/Knowledge in coding

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67-FA(PW)	FA	wangikar@iitb.ac.in	Pramod Wangikar	Metabolomics-based analysis of biochemical response to marathon running and endurance exercise	Rising awareness about the benefits of regular physical activity in reducing the risk of chronic diseases has led to significantly increased participation in endurance events such as marathons. Such intense exercise is associated with substantial changes in the energy metabolism, which improves health and endurance but may also cause deleterious effects when performed at high intensity and volume. Metabolomics analysis can highlight the alterations in metabolite levels in response to marathons, consequently identifying specific biomarkers that can help predict susceptibility to injury, assess athlete performance, and expedite the recovery process. The work will involve LCMS and GCMS based analysis of serum metabolomes of marathon runners to explore the acute metabolic perturbations associated with the exercise and subsequent recovery. The resultant data would be further used to develop a standardized test directed toward refining diet and exercise protocols to optimize the potential health benefits. This project is in collaboration with Dr. Aashish Contractor (Consultant, Center for Rehabilitation Medicine and Sports Medicine, Reliance Foundation Hospital), Dr. Marcus Ranney (Founder and CEO, Human Edge) and P. Venkatraman (Founder, You too can Run).	Metabolomics, LCMS, GCMS	Experimental	Biochemistry, Biotechnology, Life sciences.
68-FA(SBN)	FA	noronha@iitb.ac.in	Santosh Noronha	Enzyme bioreactors	The objective is to design and implement catalytic bioreactors. Work elements will involve standardization of a catalytic system, characterization of kinetic and transport aspects, process optimization, and detection in real time.	Bioreactor	Includes both, experiments and modeling	Exposure to process reaction engineering and/or biocatalysis would be an advantage.
69-FA(JS)	FA	jyotiseth@iitb.ac.in	Jyoti R Seth	Three-dimensional Self Assembly of Graphene	Three-dimensional (3D) graphene is known to have numerous applications as adsorbent, catalysts, sensors, energy storage such as batteries and super-capacitors. Further, 3D graphene is easy to handle and convenient to load as adsorbent in a packed bed. One of the ways of preparing 3D graphene is through reduction of 2D graphene oxide particles which leads to self-assembly of the reduced graphene particles in to a 3D "house of cards" type structure. However, this resultant structure has to have mechanical strength as well as flexibility and compressibility so that it is amenable to be used as packing in large scale industrial columns. At the same time, the surface area of the original 2D graphene oxide must be preserved, to the extent possible, so that the properties of 2D graphene such as conductivity and surface area are conserved. The aim of this PhD topic would be to develop techniques for preparation of 3D graphene in order to achieve desired characteristics as mentioned above. Influence of methods of reduction, types of reducing agents, kinetics of reduction and various other parameters on the number as well as strength of connections between reduced graphene particles will be studied. The dynamics of the self-assembly will also be studied through an analogous experimental system involving 3D printed sheet-like particles representing graphene. Embedded magnets in the particles will be used to tune particle-particle attraction. This work is in collaboration with Dr. Per Loethman of Foviatech GmBH (https://www.foviatech.com). The selected student may spend some time at our collaborator's lab in Germany. A collaboration with University of Delft in Netherlands is also foreseen. Further information can be found on https://www.che.iitb.ac.in/phd-ta-topic/three-dimensional-self-assembly-graphene	3D graphene	Includes both, experiments and modeling	Chemical Engineering, Chemistry, Physics
70-FA(JS)	FA	jyotiseth@iitb.ac.in	Jyoti R Seth	On-demand Jet Propulsion Fuel with High Solid Loading	A jet propulsion fuel containing suspended oxidizable nanoparticles has enhanced energy density than regular fuels. This is because the maximum calorific value of conventional jet propulsion (JP) fuels cane be as high as 36,000 MJ/m3. Addition of oxidisable nano particles with a calorific value of 136,000 MJ/m3 can yield multi-fold increase in the energy release per unit volume of fuel. However, creating stable suspensions of nanoparticles in the organic JP fuel medium is challenging as the particles quickly aggregate and settle causing failure in the propulsion system. Our lab has developed a novel method for (patent pending) for creating stable gelled propellant fuel. These suspensions are solid like at rest but flow freely as liquids under small applied pressures. The viscoelastic properties of the suspension are designed for easy use as an "on-demand" propellant fuel and with increased flight performance of the propulsion vehicles. This PhD project is aimed at developing an understanding of the rheological properties, flow behaviour and combustion properties of these fuels while implementing a process based on the lab scale protocol for bulk manufacturing of the gelled propellants, for their ultimate utilisation in a combustion set-up.	High energy density fuels	Includes both, experiments and modeling	Chemical Engineering, Chemistry, Physics

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	71-FA(OM)	FA	ojus@iitb.ac.in	Ojus Mohan	Combined Experimental and Computational Investigation of Greenhouse Gas Adsorption on Biochar	Biochar, a carbon-rich product of the thermochemical conversion (such as pyrolysis) of biomass and organic waste, has been recognized as a scalable, carbon dioxide removal technology by the United Nations Intergovernmental Panel for Climate Change (IPCC). With its high surface area, biochar can adsorb a wide range of green house gas (GHG) molecules, and its properties, such as porosity and functional groups, can influence its ability to do so. However, the adsorption mechanism of GHGs on biochar is not fully understood. The aim of this project is to investigate the potential of biochar as a sorbent for greenhouse gases (GHGs). The project will involve a combination of experimental and computational techniques (quantum mechanical simulations) to study the adsorption behavior of GHGs on biochar. The experimental part of the project will be co-supervised by Prof. Anjali Jayakumar from Newcastle University and will be done with close collaboration with the UK Biochar Research Centre at University of Edinburgh. [15]	Adsorption	Includes both, experiments and modeling	
	72-FA(SMM)	FA	sanjaym@iitb.ac.in	Sanjay M Mahajani	Value added products from non-centrifugal sugars	The project involves investigation of use of non-centrifugal sugars (jaggery) in various value-added products. NCS is a nutritious sweetener and replace white sugars in various confectioneries. The studies will cover, determining the nutrition profiles of the products, accelerated shelf life, sensory evaluation. Human trials and cell line studies will also be performed at a later stage.	Product development	Includes both, experiments and modeling	