Department of Chemical Engineering, IIT Bombay.
Preference for TA, TAP and FA Ph.D Topics for Autumn, 2020
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Sl. No. of the topics	Name & email of faculty	Title:	Objectives (4-5 lines):	Nature of the project (Experimental/ Modeling/Theoretical/):	Type of the project (TAP, TAP or FA, FA only)	Background required (e.g. Chemical Engg/Chemistry/Physics, Specific experimental expertise/Knowledge in coding etc.):
1(TA)			(Guide and topic will be decided after one semester based on the availability of the topics and positions with the faculty)			
2(GK)	Guruswamy Kumaraswamy	Structure and water transport through block copolymers with a hydrophilic block	Block copolymers are polymers comprised of "blocks" of different monomeric units connected together. This project is focused on investigations of block copolymers with glassy styrenic blocks connected to hydrophilic sulphonated blocks. Such block copolymers form films with microphase separated structure, characterized by length scales of the order of tens of nanometers. This project will investigate the structure of these block copolymers at different levels of hydration and seek to understand the forces that drive structure formation. This project will involve extensive experimentation to characterize structure, including small angle Xray scattering and, most likely, electron microscopy. Water transport will be characterized and will be modelled and correlated with the experimentally obtained structural information. Strong collaborations with industry are envisaged as part of this work.	Includes both, experiments and modeling	TAP or FA	Chemical Engineering, Research Experience using Materials Characterization is preferrable
3(KVV)	K V Venkatesh venks@iitb.ac.in (co-guide: Prof. Puruwar, BSBE)	System biology of keratinocytes - modeling and experimental studies	The project deals with omics data generation for several physiological states of keratinocytes (primary skin cells). The omics data generated will be integrated and analyzed using system level models. Both dynamical and steady state analysis will be carried out on the system. Metabolomic and proteomic data will be used in the study to enumerate the physiological states due to specific perturbations such as due to an active ingredient or due to signaling perturbation.	Includes both, experiments and modeling	TAP or FA	Biotech, systems biology, chemical engineering
4(JP)	Jason Picardo (jrpicardo@che.iitb.ac.in)	Fluid Mechanics of Mucus in Lung Airways	The small tubular air capillaries within our lungs contain a thin liquid lining of mucus. Under healthy conditions, this mucus layer is responsible for trapping and removing dust and pathogens. However, if this layer becomes too thick due to, for e.g., airway constriction and mucus over-secretion in asthmatic patients, then the airway can be choked off. The goal of this project will be to develop a fundamental understanding of lung mucus dynamics, by building and analysing a novel mathematical model, which incorporates for the first time the interaction of the mucus film with the airway wall and the core airflow [https://www.che.iitb.ac.in/group/picardo-group/article/project-openings].	Theoretical/Computational	TAP or FA	Fluid mechanics, Interest in mathematical modelling and simulation
5(AS)	Arindam Sarkar (a.sarkar@iitb.ac.in)	Electrochemical reduction of CO2 to chemicals	The project concerns development of catalysts for electrochemical reduction of CO2. The scope of work includes synthesis and characterization of catalysts and electrochemically evaluate them for reduction of CO2. Further, modification of membranes and development of a fuel cell type device for the large scale synthesis of the reduction products. Another advanced aspect would be to explore photo-electrochemical conversion of CO2 and modification of membranes for selective transport of ions. The work is largely experimental in nature involving extensive electrochemistry, and material synthesis and characterization.	Experimental	TAP	Chemical Engg, Chemistry, materials Science. Knowledge of electrochemistry, material synthesis and characterization is desired.
6(DVK)	Devang Khakhar (khakhar@iitb.ac.in), Partha S. Goswami (psg@iitb.ac.in)	Analysis and optimization of particle grinding in a spiral air jet mill	Particle size reduction is a highly energy intensive operation and even small improvements in efficiency can result in significant energy savings. The focus of the present work is analysis and optimization of an air jet mill, which is a versatile equipment used in many industries for fine grinding of powders to sizes less than around 10 microns. The objective of the project is be to develop a detailed simulation model using computational fluid dynamics (CFD) and the discrete element method (DEM).	Theoretical/Computational	TAP	Chemical Engineering

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7(AbM)	Abhijit Majumder, abhijitm@iitb.ac.in	Development of a microfluidic based tool for assessing placental functions and evaluating its potential application in pregnancy related disorders	India has a high burden of pregnancy-related complications like preeclampsia and gestational diabetes that lead to feto-maternal morbidity and mortality. Many of the pregnancy-related complications are due to placental dysfunctions. Presently, diagnostic and therapeutic research to study placental (patho-)physiology is impeded due to the lack of an appropriate model system. Here, we aim to develop a placenta-on-chip microfluidic platforms that will mimic the human feto-maternal interface. We will engineer polydimethylsiloxane (PDMS) microfluidic device to co-culture fetal and maternal cells in a matrigel in a spatial manner resembling human placenta. For device validation, we will analyse its permeability conditions and hormone secretions. To mimic blood flow conditions and preeclampsia, the effects of shear stress and increased pressure on cell migration, viability, gene expression, and placental permeability will be analysed. To mimic gestational diabetes, the effects of high glucose on expression of relevant genes and placental functions will be analysed. Transport of glucose and other molecules across the placental barrier will be estimated. Toxicity of the selected drugs on cell viability and placental permeability will be assessed.	Experimental	TAP	Previous experience of microfabrication/microfludics, cell culture
8(BKS)	Bharatkumar Suthar	Measuring spatial inhomogeneity in porous electrodes for electrochemical energy storage systems	1. Development of an experimental setup to probe local transport resistance of a porous electrode for Li-ion battery. 2. Development of data analysis methodology to extract local transport parameters. 3. Numerical simulation on the 3D reconstruction of the FIB-SEM data and the validation of numerical algorithms. 4. Perform Experiments to quantify the effect of inhomogeneity on the capacity fade of a battery electrode.	Includes both, experiments and modeling	TAP or FA	Chemical Engg, knowledge in coding and math will be helpful.
Only those candidates who have external fellowsip/s like CSIR/DBT JRF, DST INSPIRE etc can opt for the following [9(JB)-34(HNN)] topis						
9(JB)	Jayesh Bellare jb@iitb.ac.in	3D scaffolds for regenerative medicine	To develop customized grafts for bone and other tissue with 3D printing and other fabrication technologies, and to develop new methods of fabrication for bio-resorbable scaffolds. To test them by physico-chemical and biological means: in-vitro in mammalian cell culture, in-vivo in small animals, and perhaps first-in-human.	Experimental	Only FA	Any background stream, preferably with knowledge of, and willingness to learn about, biomaterials and their characterization by microscopy and related tools, mammalian cell culture, small animal studies, 3D printing, model-building in CAD packages like AutoCAD, SolidWorks, and coding in python.
10(SBN)	Santosh Noronha noronha@iitb.ac.in	Development of novel fungal expression platforms	The work involves development and characterization of targeted genome editing tools for 2 industrially important fungal species, and expression of biotherapeutics using these systems.	Experimental	Only FA	Candidates with M.Sc., or M.Tech Biochemistry, Life Sciences, Biotechnology or equivalent. Project-related experience with biochemistry, microbiology and molecular biology techniques would be an advantage.
11(SBN)	Santosh Noronha noronha@iitb.ac.in	Catalytic microreactors	The objective is to design and implement catalytic microreactors. Work elements will involve standardization of a catalytic system, characterization of kinetic and transport aspects, process optimization, detection in real time.	Includes both, experiments and modeling	Only FA	Exposure to process reaction engineering and catalysis would be an advantage.

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12(SBN)	Santosh Noronha noronha@iitb.ac.in	Production of chiral pharma intermediate(s)	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.	Experimental	Only FA	Candidates with M.Sc., or M.Tech Biochemistry, Life Sciences, Biotechnology or equivalent. Project-related experience with biochemistry, microbiology and molecular biology techniques would be an advantage.
13(JA)	Jhumpa Adhikari	Understanding phase equilibria in gas hydrates using molecular simulations	L-H. L-H-V, I-H-V phase equilibria prediction Gain insights into molecular level phenomena Study of pure and mixed hydrates	Theoretical/Computational	Only FA	Coding skills, Experience with use of open source software packages such as MCCCS Towhee, LAMMPS, GROMACS, etc.
14(SS)	Supreet Saini	Theoretical investigations into differential trait exhibition by males and females of the same species.	Two sexes of a species exhibit often different features (other than the sexual organs). For example, a peacock has a colored plume, whereas a pea hen doesn't. Often this differential manifestation of features is beneficial for the species. However, how is this phenomenon maintained in a species, when genes from males and females are mixed while mating? In other words, how to produce two different features/phenotypes, using a "shared" set of genes? Investigation of the genetics of maintenance of sexual dimorphism is the goal of this project.	Theoretical/Computational	Only FA	Any background with a strong interest in theory.
15(SS)	Supreet Saini	How does one specie split into two?	If in a population, a male and a female can mate to produce a fertile offspring - the two parents are said to be from the same species. For example, a horse and a donkey mate to produce a sterile mule - hence, horse and donkey are separate species. When a population of one species, splits into two distinct species - is called a speciation event. In this project we are interested in understanding the theory of genetics & evolution which explains speciation events in ecological settings.	Theoretical/Computational	Only FA	Interest in biology and theory.
16(MukT)	Mukta Tripathy	The phase behavior of connected hard and soft particles.	A surprising new development in materials science and chemical engineering is the finding that mixtures of hard (colloidal) and soft (polymeric or micellar) particles can self organize in long length scales. This kind of self assembly has applications in making tunable and thermo-responsive as well as pressure responsive materials that are useful in sensors, etc.In this project we explore the behavior of connected hard- and soft particles. Objectives: 1) Developing very simple models of connected hard and soft particles. 2) Determining the structure and thermodynamic properties of such particles.	Theoretical/Computational	Only FA	Chemical Engg/Chemistry/Physics background. Some knowledge of coding.
17(MukT)	Mukta Tripathy	Thermodynamic study of polymer-grafted nanoparticle composites	Grafting polymer to the surface of nanoparticles can result in enormous property enhancements. This project involves the study of thermodynamic properties of such composite systems. The topic lies in the area of polymer physics. The objectives of this project are as follows. 1) Building simple models for polymer-grafted nanoparticles. 2) Determining the structure of garfted nanoparticles in pure form, in solvent and/or in polymer matrix.	Theoretical/Computational	Only FA	Chemical Engg/Chemistry/Physics background is required. Some coding knowledge is required.
18(MukT)	Mukta Tripathy	The role of shape in the self-assembly of polymer-grafted nanoparticles	Traditionally self-assembled structures are formed using chemical differences within a species. Examples of this are the formation of micelles by detergents and the formation of the phospholipid bilayer of the cell membrane. In these systems it is the tendency to the hydrophobic and hydrophilic part to avoid each other that result in the self-assembled state. However a recent study (http://pubs.rsc.org/en/content/articlehtml/2017/sm/c7sm00230k) has pointed out that it is possible to form self-assembled states without any chemical differences. Rather it is possible to form such structured self-assembled states simply due to the shape of the nanoparticle and attached polymer species. In this study we will study how the shape of species can influence their self-assembly.	Theoretical/Computational	Only FA	Chemical Engg/Chemistry/Physics background is required. Some coding knowledge is also essential.

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19(MukT)	Mukta Tripathy	The role of impurities in the self-assembly of polymer-grafted nanoparticles.	Traditionally self-assembled structures are formed using chemical differences within a species. Examples of this are the formation of micelles by detergents and the formation of the phospholipid bilayer of the cell membrane. In these systems it is the tendency to the hydrophobic and hydrophilic part to avoid each other that result in the self-assembled state. However a recent study (http://pubs.rsc.org/en/content/articlehtml/2017/sm/c7sm00230k) has pointed out that it is possible to form self-assembled states without any chemical differences. This project focuses on how the presence of small amount of impurities (without any chemical difference from the main species) can change the self-assembly.	Theoretical/Computational	Only FA	Chemical Engg/Chemistry/Physics background is required. Some coding knowledge is essential.
20(SRJ)	Sameer Jadhav, Ganesh Viswanathan, srjadhav@iitb.ac.in, ganeshav@iitb.ac.in	Construction and analysis of signalling network governing sperm selection for fertilization	Sperm homing to the egg is a critical process in reproduction. On display is not only the ability of the sperm to swim and steer in response to fluid flow, thermal and chemical gradients, but also to compete among several million sperm cells. We and others have developed tools to observe and quantify sperm response to gradients of certain signalling molecules present in the oviductal fluid. However, the molecular pathways involved in regulating fitness of these sperm to effect fertilization remain an area of active study. The objective of the project is to construct and analyse the signalling network that regulates sperm selection during fertilization process. The project is computational and the candidate should have a background in biotechnology/bioinformatics.	Theoretical/Computational	Only FA	Biotechnology/bioinformatics
21(GAV)	Ganesh Viswanathan	Modeling phenotype switching during Tumor Necrosis Factor alpha signaling	Tumor necrosis factor alpha (TNFa), a pleiotropic cytokine is implicated in several pathological conditions. 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 pro-survival or apoptotic or necroptotic state. A detailed understanding of the intracellular state that may lead to switching between different phenotypes can offer insights on modulating the cellular response to TNFa. The objective of the project is to construct systems biology based model of the TNFa signal transduction network -- already available in PIs lab -- 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 from literature.	Theoretical/Computational	Only FA	Chemical Engg/Physics with strong interest in biology, Biotechnology. Basic knowledge in coding.
22(PW)	Pramod Wangikar (wangikar@iitb.ac.in)	Deep learning methods for human metabolomics and precision medicine.	Metabolomics, or the study of all cellular metabolites, promises to be a new cornerstone in disease diagnosis and precision medicine. Several recent reports demonstrate that metabolite profiles are excellent indicators of the health status of individuals. In addition, metabolomics monitoring is likely to be included in the clinical trials on a routine basis. However, the field of metabolomics is not nearly as developed as proteomics or transcriptomics. Identification and quantification of a large number of metabolites is a challenge. An important obstacle is that currently available data analysis tools result in a large number of false positives and thus demand significant manual curation of the results at the hands of the expert scientist. Our goal will be to develop deep learning algorithms for LC-MS/MS data analysis by employing the latest neural network techniques. This will dramatically reduce the false positives and lead to new biological discoveries. The student will reanalyze the data available in the public domain as well as the data generated within our own lab. During the initial years of PhD, the student will be expected to develop significant expertise in machine learning techniques, Python and other libraries. Basic proficiency in mathematics and programming is expected.	Theoretical/Computational	Only FA	Basic proficiency in mathematics and programming is expected.
23(PW)	Pramod Wangikar (wangikar@iitb.ac.in)	Topic 2.Development of Cyanobacterial metabolome and fluxome database (CMFD)	This initiative involves the development of the CMFD along the lines of HMDB (Human Metabolome Database). Cyanobacteria are gaining importance both as hosts for photoautotrophic production of chemicals and as model systems for studies of diurnal lifestyle. Metabolic engineering and other studies of cyanobacteria are expected to benefit from the new knowledge of metabolomics and fluxomics. However, the rapidly accumulating results of this field are not organized properly. In the present project, we will go one step ahead of the HMDB and develop a cyanobacteria specific database of the metabolites, the metabolic networks and most importantly the reaction rates of fluxes through these networks. During the initial years of PhD, the student will be expected to learn the various computational aspects such as database structure, data analysis, metabolic modeling and text mining (to include extracted knowledge from literature into the database). Basic proficiency in mathematics and programming is expected.	Theoretical/Computational	Only FA	Basic proficiency in mathematics and programming is expected.

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24(PW)	Pramod Wangikar (wangikar@iitb.ac.in)	Topic 3: Non-stationary 13C-Metabolic flux analysis of cyanobacteria.	13C-MFA helps quantify intracellular reaction rates by recursively fitting experimentally observed patterns of 13C isotope labeling of metabolites. There are two broad categories of 13C-MFA: (i) Stationary 13C-MFA that requires metabolic and isotopic steady state and (ii) Non stationary 13C-MFA that makes the use of systems that are in metabolic steady state but in a state of transition in terms of isotope labeling. Although experimentally and computationally more challenging, the non-stationary 13C-MFA is emerging as a preferred tool to probe cellular metabolism. The method provides a better resolution of the reaction rates with the ability to map a much bigger part of the network. In our group, we have developed a novel pipeline for the collection of labelling data for over 100 metabolites and fragments using LC/MS/MS. While E coli and yeast are the conventional model organisms with several applications in biotechnology, a number of non-model organisms have emerged with novel applications. The proposed work therefore involves improvement of this pipeline and 13C-MFA of non-model organisms such as cyanobacteria. The work will provide insights into (i) the overall energy efficiency of the metabolic network, (ii) flexibility at branch points in the network, and (iii) carbon overflow mechanism. The work becomes a precursor for classical metabolic engineering. During the initial years of PhD, the student will be expected to learn the various computational aspects such as metabolic modeling and flux analysis. Basic proficiency in mathematics and programming is expected.	Theoretical/Computational	Only FA	Basic proficiency in mathematics and programming is expected.
25(SMe)	Sarika Mehra, sarika@che.iitb.ac.in	Characterization of novel efflux pumps and their resistance mechanisms	Efflux pumps are one of the major determiners of resistance to antibiotics. However, predicting substrates of these pumps from the gene sequence is challenging. In this project, we will characterize novel efflux pumps, that have low sequence identity to any well characterized efflux pump, naturally present in soil species, Streptomyces to identify the key residues that provide substrate specificity. The project will be mostly experimental in nature.	Experimental	Only FA	experience in molecular biology will be beneficial.
26(RB)	Rajdip Bandyopadhyaya, rajdip@che.iitb.ac.in	Chemical sensor development for water quality parameters and contaminants	Continuous monitoring of water quality parameters, like dissolved solids, metals, ions (arsenic, fluoride etc.), organics (phenol) is an important measurement, to ascertain quality and use of a water body, whether a flowing water-stream or a stagnant water-pool, like a lake. To that end, we will work on a coated nanoparticle mediated, optical-spectra based sensor (developed by us), which has been partially tested with both synthetic and field-water samples. The aim is to further develop the nanoparticle sensor solution and study the material and interfacial properties of the sensor with contaminants in water, so as to have a functional sensor, suitable for field testing. Currently our sensors have been interfaced with automated sampling systems with data-cards for parameter monitoring. Further work on circuits and systems is needed to make it remotely functional too. Part of the work will be in collaboration with Electrical Engg. dept.	Experimental	Only FA	Chemical Engg., Electrical Engg./Electronics with some chemistry/materials background
27(RB)	Rajdip Bandyopadhyaya, rajdip@che.iitb.ac.in	Modeling and simulation of functional nanoparticles	Nanoparticles and their clusters show new and interesting properties different from bulk materials due to their extremely small size (diameter) and large specific surface area. It is thus critical to understand the variables that control its formation leading to a desired property. Control of nanoparticle size, size distribution and particle-cluster formation is the first step in all these applications. To gain further insight into the mechanism of formation of nanoparticles and its clusters, we will first look at the way individual nanoparticles form by processes like mass transfer, reaction, nucleation, Brownian collision, surface growth, coagulation and Ostwald ripening, followed by interparticle forces leading to clusters of particles.

With the mechanism in place, we will build on our existing mathematical models and computer simulation programmes, and may also carry out some small experiments, involving complex nanostructures, like core-shell nanoparticles, nanorods to validate these models. Thus, one can do computational research (using population balance or kinetic Monte Carlo) with some experiments. | Theoretical/Computational | Only FA | Chemical Engg., Physics, Computational Chemistry, Computational Materials Sc. |
| 28(AtqM) | Ateeque Malani malani@che.iitb.ac.in | Simulation Studies of Enhanced Oil Recovery | In the secondary and tertiary phase of oil recovery the crude oil in direct contact with mineral surface needs to be displaced using external medium mostly water. The mechanism of replacement is governed by the structural and energetic behaviour of interfacial water versus hydrocarbon oil at the mineral surface. This project is aimed at understanding the interfacial behaviour of crude oil-water at mineral interface. The obtained understanding will be used to enhance the oil recovery. | Theoretical/Computational | Only FA | Chemical/Chemistry/Physics/Material Science |

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29(HN)	Hemant Nanavati, hnanavati@che.iitb.ac.in	Ab initio protein structure prediction	Ab Initio protein structure prediction methods (prediction of the 3-D molecular structure using the knowledge of only the amino acid sequence) have exhibited considerable promise in the recent past with several methods, being successful in community-wide experiments (CASP). We have formulated the protein-folding problem as a combinatorial optimization problem where, a variant of Monte Carlo Minimization Algorithm has been employed to achieve the minimum energy configuration. The search for the optimum has been simplified by incorporating the various geometrical constraints of the secondary structural elements using a distance restraint potential function. Additionally, the sample space has been reduced by considering the probability distribution of backbone torsions observed in nature. Simulations carried out on a sequences varying from 29 to 85 amino acids belonging to all classes, have exhibited positive results, and indicate that large proteins can be simulated by this approach in the future in the project offered at the doctoral level.	Theoretical/Computational	Only FA	MTech/ME in ChE Materials, MSc in Physics
30(HN)	Hemant Nanavati, hnanavati@che.iitb.ac.in	Synth., Value--Addn and Processing of Biodegradable Poly(L--lactic acid) Nanocomposites, with Cellulosic ("Green") Nanofillers	Based on the Patent Applications submitted by our group for high Mol Wt. PLLA Nanocomposites with Clay Nanoparticles, we will be embarking on the challenge of incorporating ecofriendly, Cellulosic Nanoparticles as Nanofillers.	Experimental	Only FA	MTech/ME in ChE Materials, MSc in Physics
31(HN)	Hemant Nanavati, hnanavati@che.iitb.ac.in	Nanoindentation and Modeling Studies of Polymers	Nanoindentation and Modeling Studies of Polymers	Includes both, experiments and modeling	Only FA	MTech/ME in ChE Materials, MSc in Physics
32(HN)	Hemant Nanavati, hnanavati@che.iitb.ac.in	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 computational and theoretical analyses of the molecular structure of the biopolymer system, and comparison with literature experimental data.	Theoretical/Computational	Only FA	MTech/ME in ChE Materials, MSc in Physics
33(HN)	Hemant Nanavati, hnanavati@che.iitb.ac.in	Elasticity Relationships for Filled Elastomers	Filled elastomers or filled rubbers have found extensive uses in industry. The fillers provide advantageous properties over unfilled systems, leading to various applications. One important property that bears investigation is the stress-strain relationship of the elastomers and its relationship to the primary molecular architecture. Experimental data and theoretical developments have been presented earlier. The current investigation aims toward a systematic study of the objective relationship between molecular structure and stress-elongation relationship. The approach involves performing rotational isomeric states - monte-carlo (RIS-MC) simulations of entire chains, in addition to theoretical development using tools such as Mathematica. The developed models will be validated using literature data as well from experiments performed during the research.	Includes both, experiments and modeling	Only FA	MTech/ME in ChE Materials, MSc in Physics
34(HN)	Hemant Nanavati, hnanavati@che.iitb.ac.in	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	Theoretical/Computational	Only FA	MTech/ME in ChE Materials, MSc in Physics