Department of Chemical Engineering, IIT Bombay.
Preference for TA, TAP and FA Ph.D Topics for Spring, 2020-2021
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Sl. No of the topics	Name & (email) of the 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(SS)	Supreet Saini (saini@che.iitb.ac.in)	Why do species form?	Why do organisms organize themselves into discrete groups called species? Is there an evolutionary pressure on organisms to evolve so as to prevent mating (exchange of genes) with other species? In this project, we will answer these questions and understand the fundamentals of a speciation process, using the yeast S. cerevisiae as a model organism. (This project is funded by DBT/Wellcome Trust India Alliance) For more information or if you have questions/doubts, please feel free to write to Prof. Saini at saini@che.iitb.ac.in.	Experimental	TAP or FA	Microbiology, Biotechnology. (Candidates with background in Engineering/Physical Sciences with a strong interest in evolutionary biology are welcome to apply too).
3 (SS))	Supreet Saini (saini@che.iitb.ac.in)	Investigation of evolutionary forces driving sympatric speciation.	A population of a single species living in an area can split into two species. Such a process is called sympatric speciation. Members of the resulting two species are thereafter incapable of mating with each other. What causes this splitting of one species into two, remains an outstanding question. In this project, using yeast S. cerevisiae as a model organism, we will investigate this question. (This project is funded by DBT/Wellcome Trust India Alliance) For more information or if you have questions/doubts, please feel free to write to Prof. Saini at saini@che.iitb.ac.in.	Experimental	TAP or FA	Microbiology, Biotechnology. (Candidates with background in Engineering/Physical Sciences with a strong interest in evolutionary biology are welcome to apply too).
4 (GK)	Guruswamy Kumaraswamy (guruswamy@iitb.ac.in)	Structure and water transport through block copolymers with a hydrophilic block	Block copolymers are polymers comprised of "blocks" of different monomeric units connected together. Block copolymers with precisely tailored molecular structure, viz. molecular weight and connectivity of the blocks represent functional materials with remarkable properties. These materials find use in challenging applications, such as membranes for separations. 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. The formation of these structures is often out of equilibrium, resulting in slow structural changes in the membrane. This impacts properties such as the membrane conductivity as well as separation ability. 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 structure will be correlated with properties, specifically, water transport. 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 Enginereering, some exposure to polymers will be good
5 (JS)	Jyoti R. Seth (jyoti@che.iitb.ac.in)	Studies in surface modification using polymers	Inorganic salt and dust particles present in water have a tendency to precipitate and deposit on surfaces. This leads to scale formation in pipelines. In applications such as laundry and dishwashing also, it is undesirable to have particles deposit on otherwise clean surfaces. Polymers, which easily undergo adsorption on surfaces, can be used to mitigate this phenomenon. This may happen via various mechanisms. For example, with polymer adsorbed on the particle, further growth of particles may be retarded. On the other hand, by choosing the right polymer, particles can be kept suspended. To effectively design such a system, one must understand the phenomena of polymer adsorption and nature of the adsorbed surface. This is the objective of this PhD position funded by DOW. Experiments will involve generation of adsorption isotherms, studying dynamics of adsorption, measurement of retardation in growth rates of adsorbed surfaces, etc.	Includes both, experiments and modeling	TAP or FA	
6 (Atq)	Ateeque Malani (malani@che.iitb.ac.in)	Molecular Simulation Studies of Enhanced Oil Recovery Using CO2 and Steam	The crude oil in direct contact with mineral surface needs to be displaced using external medium (solvent + additives) in the secondary and tertiary phase of recovery. The mechanism of replacement is governed by the structural and energetic behaviour of interfacial system (solvent + additives + hydrocarbon oil) at the mineral surface. This project is aimed to study oil displacement capacity of CO2 and Steam using molecular simulations. Students with strong motivation for research, maths, chemical engg/chemistry and coding are encouraged to apply.	Theoretical/Computational	TAP or FA	Chemical Engg/Petrochemical/Chemistry/Physics/ - Students with strong a) motivation for research, b) background in maths, c) chemical engg/chemistry and d) coding are encouraged to apply.
7(SMM)	Sanjay Mahajani (sanjaym@iitb.ac.in)	Process development for non-centrifugal sugar (NCS) or jaggery	IITB is working on a government sponsored umbrella project to uplift the jaggery business in India making it profitable and sustainable thereby creating a promising livelihood option for farmers. There is a team working on it and a new startup is formed to commercialize the research findings in the project. The Ph. D. project involves understanding the science behind the clarification and crystallization steps in the production of NCS (jaggery). It further involves designing and commissioning of a clarifier and crystallizer in the existing pilot plant built by IITB research team in Warnanagar, Kolhapur. Several experiments will be performed to examine the effect of different parameters such as cooling policy in crystallization, and temperature and dosages of additives in clarification. Student will get involved in the modeling aspects as a part of the ongoing project.	Includes both, experiments and modeling	TAP or FA	

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8(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
Only those candidates who have external fellowsip/s like CSIR/DBT JRF can opt for the following [9(SS) to 28(AKS/AC] topis						
9(SS)	Supreet Saini (saini@che.iitb.ac.in)	Factors responsible for evolution of sexual reproduction.	In sexual reproduction, half the population does not bear offsprings. Thus, the growth of a population is reduced compared to a scenario if everyone in the population could reproduce. This phenomenon is referred to as "two-fold cost of sex". This implies that there must have been strong forces which lead to evolution of sexual reproduction, as the predominant more of reproduction among complex eukaryotes. In this project, we will explore this question experimentally using yeast S. cerevisiae - which can reproduce sexually as well as asexually.	Experimental	Only FA	Microbiology/Biotechnology (Engineering/Physical Sciences candidates with a strong interset in evolutionary biology are welcome to apply too).
10(SS)	Supreet Saini (saini@che.iitb.ac.in)	Investigation of forces leading to evolution of sexual reproduction and speciation.	Evolution of newer species from existing ones (a process called speciation) was referred to as the "mystery of the mysteries" in the 19th century. Despite more than 150 years since Darwin's Origin of Species, how and why newer species come into being has largely remained a mystery. In this project, we will investigate theoretically, the genetics and dynamics of evolution of sexual reproduction and of arrival newer species. This is important from the context of biodiversity of life on Earth, specially in a time when species are going extinct at an unprecedented rate.	Theoretical/Computational	Only FA	Biotechnology/Engineering/Physical Sciences
11(JB)	Jayesh Bellare (jb@iitb.ac.in)	Nanomedicines in zebrafish models	To develop zebrafish based models for understanding action of nanomedicines. To test them by physico-chemical and biological means: in-vitro in mammalian cell culture, in-vivo in small animals and fish, and behavioral studies. Studies will include medicines across multiple systems of medicine and mainly experimental with some model building and simulations.	Includes both, experiments and modeling	Only FA	Any background stream, preferably with formal knowledge of, and willingness to learn more about biology (including cell biology), 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.
12(SBN)	Santosh Noronha (noronha@iitb.ac.in)	1. Catalytic bioreactors	The objective is to design and implement catalytic bioreactors. Work elements will involve standardization of a catalytic system, characterization of kinetic and transport aspects, process optimization, and detection in real time.	Includes both, experiments and modeling	Only FA	Chemical Engg, Biotechnology, Life sciences.
13(SBN)	Santosh Noronha (noronha@iitb.ac.in)	Development of secretory expression platforms	The work involves development and characterization of bacterial systems for enhanced secretory production of recombinant proteins.	Includes both, experiments and modeling	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.
14(JA)	Jhumpa Adhikari (adhikari@iitb.ac.in)	Phase behaviour of clathrate hydrates using molecular simulations	Clathrate hydrates (such as methane hydrates) which occur in nature (e.g. in the permafrost region and sea floor) are a potential source of natural gas and exploitation of this resource will allow us to meet future energy demands. Further, carbon dioxide, a major greenhouse gas, may also potentially be sequestered in the form of clathrate hydrates. Molecular simulations can be employed to study the thermodynamics of the phase behaviour of these clathrate hydrates as well as gain insights into the underlying molecular level behaviour.	Theoretical/Computational	Only FA	Chemical Engg/Chemistry/Physics/Materials Science Knowledge in coding will be useful

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15(JA)	Jhumpa Adhikari (adhikari@iitb.ac.in)	Molecular Simulation Study of the Phase Behaviour of Complex Compounds in Advanced Biofuels	A molecular simulation study of the phase behaviour of the complex organic compounds present in advanced biofuels (the second generation biofuels derived from lignocellulosic biomass) is necessary as lignocellulosic biomass is a renewable, environment friendly and readily available alternative in our agrarian society to fossil fuels. Understanding the phase behaviour of advanced biofuels is important in the process modelling, simulation and optimization of industrial separation processes involving 'bio-refininig'. As many of the compounds in these biofuels decompose at elevated temperatures, experimental studies may be difficult and expensive or unfeasible and hence, we use molecular simulation techniques which are a cost effective tool to predict phase equilibria data of the individual components as well as their mixtures, and also to understand the microscopic origins of the observable macroscopic properties.	Theoretical/Computational	Only FA	Chemical Engg/Chemistry/Physics/Materials Science Knowledge in coding will be useful
16(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 minimize 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.
17(PW)	Pramod Wangikar (wangikar@iitb.ac.in)	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.
18(PW)	Pramod Wangikar (wangikar@iitb.ac.in)	Human metabolomics for 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. Most of these reports are with Caucasian patients with almost no data available for the Indian population. Furthermore, 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. Our objective is to identify intracellular metabolites as biomarkers for diagnosis and prognosis of disease in the Indian population. In the present project, we will perform metabolomics experiments on diabetic and pre-diabetic patients and healthy controls. In addition, samples and data will be obtained from the UK Biobank and the Swedish twin registry. The data will be collected with the high resolution LC/MS/MS available in our lab. The work will involve extensive data analysis and multivariate statistical analysis.	Includes both, experiments and modeling	Only FA	Involves experimental work, design of experiments and LC/MS data analysis. Candidate should preferably be M Sc or B Tech in chemical engineering, biotechnology, life sciences or biochemistry.
19(RB)	Rajdip Bandyopadhyaya (rajdip@che.iitb.ac.in)	Real time water quality monitroing by on-board sensor development and implementation	Objective of the project is to monitor physical, chemical and biological parameters of a water source, by developing and integrating new and existing sensors, respectively. These sensors are based on our laboratory-synthesized nanomaterials and are to be explored for sensitivity, selectivity and storage stability. It is a joint collaborative project with other engineering depts. and external organization.	Experimental	Only FA	Chemical Engg., Chemistry, Materials, Nanoscience, Electrical/Electronics
20(RB)	Rajdip Bandyopadhyaya (rajdip@che.iitb.ac.in)	Functional Nanoparticles: Experiments, modeling, simulation	Objective of the project is to explain anisotropic nanoparticles synthesized in our laboratory. One has to explore new techniques to model, from spherical to conical, and finally to cylidrical transforamtion, of a initial pair of nanoparticles. It will be based on our existing models of growth of nanoparticles by different modes and validating it with further new experiments. Finally, nanorods can be used for various applications in sensors, water treatment and drug delivery, as per prevailing interst in our research group.	Includes both, experiments and modeling	Only FA	Chemical Engg., Physics, Chemistry, Materials, Nanoscience
21(SMe)	Sarika Mehra (sarika@che.iitb.ac.in)	Regulation of efflux pumps in drug resistant Mycobacteria	Multiple efflux pumps are overexpressed in clinical strains of resistant Mycobacterium tuberculosis. In this project, we aim to identify and characterize the regulatory mechanisms behind this over-expression and its role in the evolution of resistant bacteria.	Experimental	Only FA	Molecular Biology

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22(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
23(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
24(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
25(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
26(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
27(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
28 (AC/AKS)	A. K. Suresh (aksuresh@iitb.ac.in) & Abhijit Chatterjee (abhijit@che.iitb.ac.in)	Direct aromatization of methane - theoretical and experimental studies	Enormous amounts of natural gas are flared every year, causing a loss of potential hydrocarbon resources and emitting hundreds of million tons of CO2 in the earth's atmosphere. If this methane were to be captured and converted into a useful liquid fuel this would be a beneficial product and also help to reduce CO2 emissions associated with natural gas processing. It is known that Mo/ZSM-5 is an effective catalyst for converting methane to aromatic products – but, unfortunately, this catalyst also deactivates readily due to coke formation. The process needs to be developed further with a view to reducing coke formation at the same time as improving reaction kinetics and maximising aromatic products, especially monoaromatics such as benzene, and alkylaromatics which are useful as fuel additives and/or as chemical precursors. This project will help develop technologies for conversion of methane to aromatic products.	Experiments and theory	Only FA	