"Department of Chemical Engineering, IIT Bombay.
Preference for TA, TAP and FA Ph.D Topics for Autumn, 2021-2022
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Sl No	Email Address	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(GK)	guruswamy @iitb.ac.in	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. 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. We 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.	Includes both, experiments and modeling	TAP or FA	Chemical Engineering or Physics
3(SS)	saini@che. iitb.ac.in	Supreet Saini	Investigation of evolutionary forces dictating sympatric speciation.	A population of one species living in a particular environment can split to becomes two distinct species. Such an event is called sympatric species. Despite being thought to be an important mode towards generating newer species, speciation via this mode has never been demonstrated. In this project, using yeast as a model organism - we aim to demonstrate sympatric speciation in a laboratory setting. Overall, this allows us to understand how newer species and diversity in life forms are created.	Experimental	TAP or FA	Any background with a strong interest in evolution, genetics, metabolism.
4(Atq)	amalani@IIT B.ac.in	Ateeque Malani (amalani@IITB. ac.in, malani@che.iitb. ac.in)	Molecular Simulation Studies of Enhanced Oil Recovery	The crude oil in direct contact with rock surface needs to be displaced using external agents (solvent + additives) termed as Enhanced oil recovery. The mechanism of replacement of oil-rock interface by solvent-rock interface is governed by the structural and energetic behaviour of oil and solvent at the rock-oil interface. This project is aimed to study oil displacement capacity of traditional solvent (water, brine) and novel (supercritical co2) solvent using molecular simulations. Student with curiosity, strong motivation to learn new things, and good mathematical skills are encourage to apply.	Theoretical/Computational	TAP or FA	BTech or MTech in Chemical/Mechanical/other Engg, MSc in chemistry/Physics/Material science
5(Atq)	amalani@iitb .ac.in	Ateeque Malani & Jhumpa Adhikari (malani@che.iitb. ac.in, adhikari@che. iitb.ac.in)	Gas hydrate formation and inhibition: Thermodynamic and Molecular Simulation Study	During transport of crude oil and gas, often gas hydrates are formed in pipelines which creates flow assurance problem. Gas hydrates are found in deep reservoirs as well. For efficient transport of crude oil, prevention of gas hydrate formation is necessary. The project aim is to understand the thermodynamics and kinetics of gas hydrate formation and prevention using external chemicals.	Theoretical/Computational	TAP or FA	BTech, MTech in Chemical/Mechanica/Petroleum and other related, MSc in Chemistry/Physics/Material Science
6(GAV)	ganeshav@ii tb.ac.in	Ganesh Viswanathan, ganeshav@iitb. ac.in	Modulation of mammalian cell signalling	Ability to modulate behaviour of enzymatic futile cycles or cascades, which are sentinels of mammalian cell signalling, can have a wide-ranging impact on the response of normal and diseased cells. Novel retroactive or reverse signalling in a futile cycle such as MAPK cascades can offer specific response modulations that are not possible otherwise. The goal of this project is to understand how downstream retroactive signalling can impact the behavior of activated MAPK cascade in myeloid lymphoma cells stimulated with TNFa. The project will involve sophisticated high-throughput perturbative experimentation at single-cell and population-averaged levels.	Experimental	TAP or FA	B.Tech/M.Tech Biotechnology or M. Sc Biological Sciences/Biotechnology.
7(GAV)	ganeshav@ii tb.ac.in	Ganesh Viswanathan, ganeshav@iitb. ac.in	Stochasticity in mammalian cell signaling	Mammalian systems are exposed to fluctuating environments at all levels making their response a chance process. The goal of this project is to distil out the effects of stochasticity in various motifs or building blocks such as enzymatic cascades, which are sentinels of cellular signalling. The project will involve developing mathematical kinetic model of biochemical reactions corresponding to these motifs. Model simulations by incorporating stochasticity will be contrasted with already generated experimental data. Student will work closely with the experimentalists.	Theoretical/Computational	TAP or FA	B.E/B.Tech/M.Tech in Chemical Engineering/Mech Engineering/Biotechnology or M.Sc Physics/Biotech.

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8(BKS)	bharat.k.suthar@iitb.ac.in	Bharatkumar Suthar	Enabling e-mobility through accurate measurement of nano-scale processes in li-ion battery	Accurate battery model is the key for designing a battery pack for e-mobility applications ensuring safe and efficient battery operations. While simplified battery models (equivalent circuit models) are desirable for control-relevant application, detailed electrochemical models which connect the dynamics at the nanoscale to the sub-mm scale (and larger) are needed for designing battery pack as well as coming up with its usage (charging/discharging) policy for long-lasting and safe battery operations. Tremendous engineering efforts at the nano-scale goes into designing battery materials that are safe and have a long life. While the general modeling frameworks incorporating the dynamics at the nano-scale are well established in literature they require a set of parameters to be accurately measured. This project relates to taking a commercial battery (where very little is known from the manufacturers), opening it up, and coming up with ways to measure as many parameters as possible. Such measurements will be electrochemical (transport properties of lithium/lithium ions in nanopores or nanoparticles), physical (size distribution, pore network, porosity, tortuosity, etc.), chemical (composition and distribution of elements in nanoparticles), thermal (heat conductivity) or electrical (resistances) in nature. Accurate measurement of such parameters will enable the development of an experimentally validated battery model of a commercial li-ion cell. Such models will be key to ensure safe and lasting battery operation as well as a detailed design of battery packs for various applications.	Includes both, experiments and modeling	TAP or FA	Chemical engineering (Transport phenomena, reaction engineering, numerical and computational methods) Both experimental and modeling components. Background in Python/Matlab/COMSOL
9(RaD)	dasgupta.ratul@iitb.ac.in	Ratul Dasgupta	CFD simulations of breaking waves and sea spray formation	This is a DST-SERB (Dept. Science & Technology) funded project aimed at studying computationally and theoretically, the breaking of waves in the ocean and the resultant spray and subsequent aerosols which are generated through this complex process. Ocean spray is produced when wind generated surface waves break and constitute an important source of marine sea salt aerosols (SSA). Many numerical models of weather require accurate estimates of the rate of generation of these aerosols under given wind conditions. The proposed Ph.D. work will study this process computationally (CFD simulations) and model it analytically to come up with accurate models of rate of generation of SSA. There will be scope to learn CFD algorithms, implement them in open source codes and participate in mathematical modelling of the fluid mechanics. Students interested in research fluid mechanics (two phase laminar and turbulent flows), computer programming and maths with strong academic background, are particularly encouraged to apply.	Theoretical/Computational	Only TAP	Chemical / Mechanical / Aerospace Engineering or M.Sc. Physics
Only those candidates who have external fellowsip/s like CSIR/DBT JRF can opt for the following topis							
10(SS)	saini@che.iitb.ac.in	Supreet Saini	Why is evolution repeatable?	The paleontologist Stephen Gould once asked if replaying evolution of life on Earth would lead to the same outcomes. While Gould's question was rhetorical, hundreds of experiments since have demonstrated a remarkable parallelism in evolutionary response of a population, when propagated under identical conditions. What causes this repeatability in evolutionary patterns? In this project, we will develop theory to answer the above question.	Theoretical/Computational	Only FA	Coursework in basic engineering mathematics and programming. A strong interest in evolution.
11(SS)	saini@che.iitb.ac.in	Supreet Saini	How do genes cross a species barrier?	Horizontal Gene Transfer (HGT), movement of genes from one species to another, is one of the major determinants of evolutionary trajectories of populations. HGT is also a strategy for heterologous protein expression in biotechnology applications. HGT However is often not successful in terms of correct expression and folding of the protein encoded. How can, then, the coding region acquire mutations and exhibit function in the new genome/species? Understanding the fundamentals of this process is the goal of this project. We will develop a rational strategy to identify mutations which facilitate successful expression of genes in a new species. The project will help enhance our understanding of evolutionary processes, and also aid heterologous protein expression for biotechnology applications.	Experimental	Only FA	Any background with a strong interest in evolution, biotechnology.

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12(SS)	saini@che.iitb.ac.in	Supreet Saini	Evolution of bifunctional proteins.	Many proteins serve more than one biological function in a cell. In fact, mutations where one of the functions is compromised are responsible for a number of diseases in humans. This means that, during evolution, these proteins must evolve to enhance a functionality, without compromising the second function. Thus, these proteins are under what is called divergent selection. How is evolution of bifunctional proteins different than a protein which serves only one function? This project is theory and bioinformatics based. Students from any background are welcome to apply. Background in biology is not required, however, a strong interest in experimental evolution, computational biology is mandatory.	Includes both, experiments and modeling	Only FA	Background in biology is not required, however, a strong interest in experimental evolution, computational biology is mandatory.
13(SBN)	noronha@iitb.ac.in	Santosh Noronha	Catalytic bioreactors	The objective is to design and implement catalytic bioreactors. Work elements will involve standardization of a catalytic system, characterization of kinetic and transport aspects, process optimization, and detection in real time.	Includes both, experiments and modeling	Only FA	Candidates with M.Tech or M. Sc. Chemical Engineering, Biochemistry, Life Sciences, Biotechnology or equivalent. Project-related experience with biochemistry, microbiology and molecular biology techniques would be an advantage.
14(JA)	adhikari@iitb.ac.in	Jhumpa Adhikari (adhikari@iitb.ac.in)	Rational design of solvents for the extraction of natural products	CAMD for task-specific solvent design Guidelines based on molecular insights obtained via molecular simulations	Theoretical/Computational	Only FA	Interest in coding
15(SBN)	noronha@iitb.ac.in	Santosh Noronha	Production of chiral pharma intermediates	The objective of this project is to overproduce a key chiral 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. Chemical engineering background candidates with project experience related to microbial biotechnology will also be considered.
16(GAV)	ganeshav@iitb.ac.in	Ganesh Viswanathan, ganeshav@iitb.ac.in	Orchestration of cancer cell response	Tumor necrosis factor-alpha (TNFa), an inflammatory cytokine present in large quantities in a tumor microenvironment, is strongly implicated in various cancer cell responses. The objective of this project is to understand the orchestration of response of cancer cells exposed to a drug cocktail. The project will involve static and discrete dynamical modelling of activated TNFa signalling network consisting of biochemical reactions, curated in-house. The focus will be on studying the effects of various cancer-specific drugs on the orchestration of TNFa network response. A combination of graph theory and machine learning algorithms will be used to achieve these objectives.	Theoretical/Computational	Only FA	B.E/B.Tech/M.Tech in Chemical Engineering/Mech Engineering/Biotechnology or M.Sc Physics.
17(SMe)	sarika@che.iitb.ac.in	Sarika Mehra, sarika@che.iitb.ac.in	Developing improved CHO host cells for production of monoclonal antibodies	Recombinant proteins such as monoclonal antibodies form a major part of the therapeutics used to treat various diseases. Mammalian cells, specifically CHO cells, are preferred as hosts for the production of recombinant therapeutics due to their ability to post-translationally modify and secrete functionally active proteins. In this project, we aim to develop a CHO host cell that is engineered to enhance its protein secretion capacity to improve the productivity of recombinant proteins.	Experimental	Only FA	chemical engg/biotechnology and related disciplines
18(SMe)	sarika@che.iitb.ac.in	Sarika Mehra, sarika@che.iitb.ac.in	Tracking emergence of resistance in Mycobacteria.	Evolution of Mycobacteria smegmatis, a model organism for understanding drug-resistant Tb, consistently results in mutations in a regulatory gene. Interestingly, the mutations are at different locations of the gene. In this project, we will track the emergence of these mutations in a population of bacteria subject to various antibiotic pressures.	Experimental	Only FA	

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19(PW)	wangikar@iitb.ac.in	Pramod Wangikar	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.	Experimental	Only FA	M Sc or B Tech in chemical engineering, biotechnology, life sciences or biochemistry.
20(HN)	hnanavati@iitb.ac.in	Hemant Nanavati	Accurate Molecular Models for Real Polymers	We develop compact, closed form, but accurate molecular models as well as elasticity relationships for real polymers, incorporating structural aspects. The applications include synthetic as well as high performance Bio-sourced polymers.	Theoretical/Computational	Only FA	Chemical Engg/Chemistry/Physics
21(HN)	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers	In this project, the aim is to understand quantitatively the molecular elasticity of biopolymers with potential engineering applications. The first example is Spider Dragline Silk, which may be several times stronger than steel (after normalizing the density). The work involves experimental, computational and theoretical analyses of the molecular structure of the biopolymer system.	Includes both, experiments and modeling	Only FA	Chemical Engg/Chemistry/Physics
22(HN)	hnanavati@iitb.ac.in	Hemant Nanavati	Multiscale Investigations on Polymeric NEMS (Nano-Electro-Mechanical-Systems)	Modeling and Experiments (Nanoindentation, etc.) on Polymeric Materials to develop an understanding of relevant aspects for NEMS Applications	Includes both, experiments and modeling	Only FA	Chemical Engg/Chemistry/Physics/Polymers
23(HN)	hnanavati@iitb.ac.in	Hemant Nanavati	Accurate Molecular Models for Real Polymers	We develop compact, closed form, but accurate molecular models as well as elasticity relationships for real polymers, incorporating structural aspects. The applications include synthetic as well as high performance Bio-sourced polymers.	Theoretical/Computational	Only FA	Chemical Engg/Chemistry/Physics/Polymers
24(HN)	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers	In this project, the aim is to understand quantitatively the molecular elasticity of biopolymers with potential engineering applications. The first example is Spider Dragline Silk, which may be several times stronger than steel (after normalizing the density). The work involves experimental, computational and theoretical analyses of the molecular structure of the biopolymer system.	Includes both, experiments and modeling	Only FA	Chemical Engg/Chemistry/Physics/Polymers
25(RB)	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Nanoparticle based composites for heavy metal remediation from water	Heavy metal in water due to industrial discharge and other anthropogenic sources causes serious health issues. In this project we will synthesize specific nanoparticles which will adsorb and react heavy metals in different ionic forms and thereby reduce their amount within allowed limits. The nanoparticles will be impregnated into fibers and packed into filter cartridges so as to design and operate devices capable of heavy metal remediation with a reasonably high throughput of treated water. There is scope of experimental and design innovation geared towards product development and also modeling to interpret adsorption and kinetics of heavy metal removal depending on background and interest of the student.	Includes both, experiments and modeling	Only FA	B.Tech. or M. Tech. in Chemical or Materials or Environmental Engg. or MSc. in Chemistry or Nanoscience and Nanotechnology
26(JB)	jb@iitb.ac.in	Jayesh Bellare	Zebrafish models for nanomedicine studies	To develop zebrafish based models for understanding action of nanomedicines including Allopathic, Ayurvedic and Homeopathic ones. To test them by physico-chemical and biological means: in-vitro in mammalian cell culture, in-vivo in small animals and fish, fish embryos, 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.

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27(JB)	jb@iitb.ac.in	Jayesh Bellare	3D printing and Simulation of resorbable occlusion devices for surgery	To develop customized devices for closing holes in hearts and other tissue repair with 3D printing and newer methods of fabrication for bio-resorbable polymers. To test them by computer simulations and by physico-chemical and biological means: in-vitro in mammalian cell culture and in-vivo in small animals, and perhaps first-in-human.	Includes both, experiments and modeling	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 Ansys, AutoCAD, SolidWorks, and coding in python.
28(JS)	jyotiseth@iitb.ac.in; vaj@che.iitb.ac.in	Jyoti Seth and Vinay Juvekar	Three dimensional graphene hydrogels: analysis of selfassembly process and environmental applications	Three-dimensional graphene hydrogels can be packed into adsorption columns for removing pollutants from wastewater or as for water disinfectants (after immobilizing silver nanoparticles on their surface). These hydrogels can be regenerated without removing them from the column and hence can be reused over multiple cycles. Focus of the present study is to understand the reduction self-assembly process in order to produce high surface area and high strength 3D graphene hydrogels. The objective also includes exploration of the applications of these hydrogels for the adsorption of aromatic pollutants (such as phenols) as well as for silver nanoparticle-mediated water disinfection.	Includes both, experiments and modeling	Only FA	Chemistry, Physics, Materials Science/Engineering, Nanotechnology, Chemical Engineering