

Ph.D. Program  
Centre for Research in Nanotechnology & Science (CRNTS)  
Indian Institute of Technology - Bombay

Topics for CRNTS Ph.D. Program (AUTUMN SEMESTER) (Dec 2023)

Candidates are encouraged to contact faculty members by e-mail directly in case they have any query.

Sr. No.	Name of Topic	Guide Name	Co-Guide Name	Category
1	Thermomechanical recycling by controlling polymer blend nanostructure	Guruswamy Kumaraswamy, Chemical Engineering guruswamy@iitb.ac.in	Debabrata Maiti, Chemistry dmaiti@chem.iitb.ac.in	TA/FA/SW/SF/IS/EX/CT
<p>Topic Name :Thermomechanical recycling by controlling polymer blend nanostructure</p> <p>Abstract :Plastic waste represents a growing challenge. Since waste streams typically comprise multiple polymers thermomechanical recycling results in blends with poor mechanical properties. This is due to the fact that polymers are typically immiscible. This can be attributed to their macromolecular nature that magnifies the contribution of monomer monomer enthalpic interactions. To upcycle the recycled blends it is necessary to control structure the polymer polymer interface. For such immiscible blends the interface is characterized by a size scale of a few nanometers and is responsible for mechanical failure of the blends. We propose to explore the use of a novel class of bisdiziridine based crosslinkers to dynamically compatibilize polymer blends by influencing the polymer polymer interface. Therefore this project will involve synthesis of suitable linker molecules as well as polymer processing to create blends and characterization of blend nanostructure using electron microscopy and SAXS.</p>				
2	Focused Ion Beam (FIB) based Defect Engineering for tuning optical and electrical properties of 2D graphene-like materials	Rakesh G. Mote, Mechanical Engineering rakesh.mote@iitb.ac.in	M Aslam, Physics m.aslam@iitb.ac.in	TA/FA/SW/SF/IS/EX/CT
<p>Topic Name :Focused Ion Beam (FIB) based Defect Engineering for tuning optical and electrical properties of 2D graphene-like materials</p> <p>Abstract :Focused Ion Beam (FIB) has emerged as a nanofabrication tool capable of resist-free, mask-less, and site-specific patterning. Recently controlling 'defects' in the materials, in the form of implantation or formation of patterns like nano-holes/channels, arrays, edges, is gaining wide attention in order to 'engineer' exotic optical properties as required by next generation application in hybrid optoelectromech and quantum devices. The project aims to systematically introduce the material defects using FIB techniques. The ion-matter interaction at the nanoscale is to be investigated in generating the defects deterministically for materials like van der Waals (vdW) materials, transition metal dichalcogenides (TMDs), etc. The FIB process is to optimized based on understanding of the ion bombardment effects and the desired spatial accuracy. The approach involves numerical studies (molecular dynamics, monte-carlo methods, etc.), FIB experimentation and advanced material characterization (SEM/TEM, AFM, etc.). The performance of such defect-engineered materials will be assessed for novel applications in integrated photonics, nanoscale/quantum sensing, quantum emitters, nanofluidics, etc.</p>				

Sr. No.	Name of Topic	Guide Name	Co-Guide Name	Category
3	Combustion dynamics of metallic nanoparticle based nanofuel spray	Abhijeet Kumar, Mechanical Engineering abhijeet.kumar@iitb.ac.in	Hrishikesh Gadgil, Aerospace Engineering gadgil@aero.iitb.ac.in	TA/FA/SW/SF/IS/EX/CT
<p>Topic Name :Combustion dynamics of metallic nanoparticle based nanofuel spray</p> <p>Abstract :Considering the decline in fossil fuel production and the increase in the price of the fuels, a need for sustainable and highly energetic fuel has emerged. In this regard, metallic nanoparticle based nanofuel appears as an excellent alternative as it possesses several benefits over traditional fuels such as high calorific value, higher thermal efficiency, reduced greenhouse gas generation and lower specific fuel consumption. Despite its potential applicability in the aviation sector, power generation systems, and supersonic aircraft, the mechanism behind the combustion behaviour of nanofuel hasnâ€™t been explored in detail. The reason behind this void is the multi-parametric influence on the nano-fuel combustion such as the particle size and mass loading of the suspended metal/metal oxide nano-particles in the base fuel, as well as the combustibility of the metal/metal oxide nano-particles. Since the efficiency of the combustion system depends on the spray quality, adiabatic flame temperature of the resulting spray flame, distribution of heat flux in the combustion chamber, and the spatiotemporal variation in the heat flux, the proposed work targets to improve the understanding of the nano-fuel spray atomization and combustion and explore the underlying spatio-temporal unsteadiness.</p>				
4	Development of photothermal catalysts for sustainable carbon dioxide conversion using solar energy	Sonali Das, Chemical Engineering sonali.das@iitb.ac.in	Debabrata Maiti, Chemistry dmaiti@iitb.ac.in	TA/FA/SW/SF/IS/EX/CT
<p>Topic Name :Development of photothermal catalysts for sustainable carbon dioxide conversion using solar energy</p> <p>Abstract :The concept of converting CO2 into synthetic fuels and chemicals using sunlight as the sole energy source holds tremendous prospects for establishing a sustainable carbon-neutral economy. Unfortunately, the light utilization efficiency of CO2 conversion via traditional photocatalytic processes, that utilize only UV/purple light, remains too low for practical use. â€œPhotothermalâ€• catalysis is an emerging field that employs plasmonic materials to utilize the full spectrum of sunlight (UV, visible, and IR spectra) and can combine both thermal and photochemical contributions of sunlight to drive catalytic reactions at unprecedented rates. However, the research area is new, and catalyst development for photothermal CO2 conversion remains in an under-utilized and rudimentary stage. The choice of appropriate catalysts is critical to ensure effective combination of light and heat to achieve practically relevant product yields under realistic sunlight conditions. Photothermal conversion of CO2 is a multi-step and multi-functional process, with various functional sites operating in tandem to harvest light and photothermally convert CO2. Intricate design and engineering of the catalyst structure and morphology at the nano scale is required to maximize the synergetic functioning of the various functional sites. The proposed research aims at developing tailor-made photothermal catalysts for light-driven CO2 hydrogenation to solar methane by engineering hierarchical carbon-containing nanostructures derived from metal organic frameworks (MOFs), that can facilitate synergistic functions of light harvesting, photon-to-heat conversion, heat retention, and CO2 activation. A primary focus of catalyst synthesis and development would be to study the effect of catalyst morphology on photothermal activity and to develop rigorous structure-property relations that can be used to develop catalysts with high solar-to-fuel conversion efficiency.</p>				

Sr. No.	Name of Topic	Guide Name	Co-Guide Name	Category
5	Defects in Semiconductor Nanodevices	Sandip Mondal, Electrical Engineering 10001970@iitb.ac.in	Prof M Maniraj, Physics maniraj@iitb.ac.in	TA/FA/SW/SF/IS/EX/CT
<p>Topic Name :Defects in Semiconductor Nanodevices</p> <p>Abstract :The revolutionary impact of advanced semiconductor physics on our daily lives remains unabated. We continually interact with computational, memory, and imaging devices where a large number of electrons are pushed around various defect states at every nanosecond inside semiconductors. As these technologies are rapidly evolving from traditional circuit boards to flexible electronics, new materials, physics, and processing technologies are being explored to improve their functionality and efficiency. This brings unique experimental challenges to evaluating the fundamental interaction of defects with electrons in novel semiconductors. In this project, we will first design a prototypical MIS capacitive device architecture to illustrate the electron trapping in memory devices fabricated at low temperatures. Unlike the conventional measurement system, we will then focus on the challenges in measuring the defect state in semiconductors and our approach to probing the defect state during charge pumping operations.</p>				
6	Nano Memory Devices for Artificial Intelligence	Sandip Mondal, Electrical Engineering 10001970@iitb.ac.in	Prof M Maniraj, Physics maniraj@iitb.ac.in	TA/FA/SW/SF/IS/EX/CT
<p>Topic Name :Nano Memory Devices for Artificial Intelligence</p> <p>Abstract :Biological neural systems can learn and forget information which is one possible mechanism for the stability and lifelong learning of neural circuits. Emulating such features in electronic devices is essential for advancing neuromorphic electronics for Artificial Intelligence. In this project, we will explore memory devices using oxides to illustrate learning behavior. We will examine the transient memory and forgetting dynamics by controlling the materials chemistry. Using examples of prototypical Mott insulators such as NiO and VO<sub>2</sub> and nanoparticles, we will present our vision for a neuromorphic platform utilizing quantum materials. Our studies will inform the design of electronic hardware in emerging Artificial Intelligence and can in the future be extended to brain-machine interfaces.</p>				

Sr. No.	Name of Topic	Guide Name	Co-Guide Name	Category
7	Developing droplet-microfluidic method to form soft nano-carriers for dual drug delivery	Venkata Ramana Gundabala, Chemical Engineering venkatg@iitb.ac.in	Sunita Srivastava, Physics sunita.srivastava@iitb.ac.in	TA/FA/SW/SF/IS/EX/CT
<p>Topic Name :Developing droplet-microfluidic method to form soft nano-carriers for dual drug delivery</p> <p>Abstract :Nanomaterials have emerged as potential candidates for research studies in all areas of science including biomedical applications such as drug delivery, diagnosis, and therapeutics. Liposomes (LP) have been considered promising and versatile drug vesicles. LPs are essentially composed of phospholipids that self-assemble to form vesicular structures in which the lipid bilayer surrounds an aqueous core. The interior of lipid bilayer and the aqueous core has been used as a carrier for hydrophobic and hydrophilic drugs respective. Compared with traditional drug delivery systems, liposomes exhibit better properties, including site-targeting, sustained or controlled release, protection of drugs from degradation and clearance, superior therapeutic effects, and lower toxic side effect. The challenges in the use of liposomes encapsulation, prepared by thin film rehydration, ethanol injection and double emulsion methods is the size polydispersity arising from inhomogeneous chemical and mechanical conditions during the mixing of bulk phase. Microfluidics has been used for manipulating micro- and nanoscale self-assembled systems with fine control over particle size and speed using a variety of fluidic materials and features. Microfluidic directed formulation of liposomes and encapsulation of proteins and drugs, has emerged as a promising alternative, which ensures precise control over the synthesis parameters, high uniformity, reproducibility, and ease of integration. Typically, a three channel microfluidic device is used for hydrodynamic focusing for the controlled self-assembly of monodisperse liposome. The streams of lipids dissolved in isopropyl alcohol is hydrodynamically focused and sheathed between two oblique aqueous buffer streams in a microfluidic channel. The laminar flow in the microfluidic channel enables controlled diffusive mixing at the liquid interfaces causing the lipids to be insoluble and self-assemble into vesicles. Microfluidics enable precise and reproducible control of the flow conditions and hence reproducible fluidic mixing on the micrometer length scale. Using this technique, the liposome size is tunable over a mean diameter of 50 nm to 150 nm by adjusting the aqueous to solvent volumetric flow rate ratio. Other existing microfluidic methods for preparation of lipid nanoparticles (LNPs) include, T or Y junction, hydrodynamic flow focusing, and staggered micromixers. The former two methods usually yield LNPs with poor monodispersity, with micromixers providing much better monodispersity. However, all these current approaches are based on 2D microfluidics that result in major drawbacks such as ineffective mixing, possibility of clogging, and being expensive. These designs generate small size liposome nanoparticles (&lt; 200nm) which limits the drug loading capacity and its application for gene therapy. In the past decade, as new drug delivery systems are emerging, encapsulating and delivering dual drugs for various diseases has garnered major attention. Dual drug delivery through a single drug delivering system can reduce drug resistance and non-specific cell toxicity, and can promote synergistic drug activity. In this project, the student will develop a droplet-based microfluidic approach to generation of double emulsion droplets that carry lipid nanoparticles to be used as dual drug (hydrophilic and hydrophobic) delivering vehicles. The generation of dual drug delivery system is achieved through controlled coalescence of the single and double emulsion droplets. The coalescence results in formation hydrophilic drug carrying LNPs in the aqueous shell with an intact hydrophobic drug carrying solvent core. 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. The liposome nanoparticles present in the shell of the generated Dual Drug Delivery System (DDDS) will be characterized using the fluorescence based imaging and high resolution synchrotron based small angle x-ray scattering (SAXS) characterization techniques. The in-situ measurements shall unravel the self-assembly mechanism during the formation of the nanoparticle-lipid complexes for improved structural stability. These studies shall allow further gaining insight into the involved dynamic structural transitions, mechanisms, and kinetics during the generation of self-assembled nanostructures (including drug nanocarriers) at different reaction times (ranging from fractions of seconds to minutes). Using the newly designed microfluidic platform the student will test the loading of hydrophilic and hydrophobic drugs into the LNP carrying double emulsions, for cancer treatment. Photo thermal and MTT essay studies will be performed for drug release and efficacy measurements.</p>				

Sr. No.	Name of Topic	Guide Name	Co-Guide Name	Category
8	Study of morphogenesis in living structures using image analysis, geometrical quantification, and theoretical modeling.	Mandar Mukund Inamdar, Civil Engineering minamdar@iitb.ac.in	Raghunath Chelakkot, Physics raghu@phy.iitb.ac.in	TAP/PS
<p>Topic Name :Study of morphogenesis in living structures using image analysis, geometrical quantification, and theoretical modeling.</p> <p>Abstract :The Form of a structure is comprised of its shape, size, internal configuration, and texture. Morphogenesis means the origin of form and involves the study of how living systems get their shape in response to their designed function. Epithelial tissues are important biophysical structures that are formed by a group of connected living cells. In this project, we will investigate how spherical epithelial tissues lose their initial shape symmetry and undergo morphological changes as a result of phenomena occurring at sub-cellular and cellular scales. At the implementation level, the project has three components. The first step involves analyzing the experimental images of tissues from our French collaborator using cutting-edge tools in image analysis and machine learning. The second step involves theoretical quantification of tissue deformation from these analyzed images using tools from computational geometry. The final step is developing a computational model to get a deeper understanding of these experimental findings and predict the mechanical behavior of the tissues. In summary, the goal of this inter-disciplinary, Indo-French project, which is at the interface of engineering, physics, and biology, is a theoretical investigation of epithelial morphogenesis in close synergy with experiments.</p>				
9	Micromechanical theory for explaining yielding phenomena in the colloidal system	Lalit Kumar, Energy Science & Engineering lalit.kumar@iitb.ac.in	Jhumpa Adhikari , Chemical engineering adhikari@iitb.ac.in	TA/FA/SW/SF/IS/EX/CT
<p>Topic Name :Micromechanical theory for explaining yielding phenomena in the colloidal system</p> <p>Abstract :Yield stress is an important concept in the real and industrial materials involving colloidal aggregates. Yield stress characterizes transition from the solid-to-fluid behaviour. However, most of the time material reaches the yield condition via elastic deformation. For a material which has varying contact surface throughout the materials, defining yield stress is even more challenging. In these types of materials, there is a continuous contact breakage until material reaches the yield point. Despite numerous availability of these types of materials, there are very few studies which try to connect microscopic property to the macroscopic mechanical response even using spherical colloidal assumptions. In this work, we want to understand the yielding process and formulate a new constitutive model for the colloidal system.</p>				