

Interdisciplinary Themes for PhD Admissions (November 2022)

Theme: Biomedical Devices Coordinator: Prof. Uttama Lahiri				
Sl. No.	Project Title	Investigators	Project Description	Minimum Eligibility requirement
1	Wearable SmartSuit for Predicting Freezing from Gait and Posture and Ensuring Uninterrupted Mobility of patients with Parkinson's Disease	PI: Uttama Lahiri Co-PI: Biswajit Saha Co-PI Manasi Kanetkar	This wearable technology with a customized data analysis system will allow patients with Parkinson's disease to predict freezing from gait.	First Class or 65% marks (60% for SC/ST/PD) or 6.5(6.0 for SC/ST/PD) CPI/CGPA on the scale of 10 in: BE/BTech/ME/MTech or Equivalent degree in the broad area of Electrical and/or Electronics engineering, OR BE/BTech/ME/MTech or Equivalent degree in other branches of Engineering may be considered in areas consistent with the research areas of the discipline, OR MSc in disciplines consistent with the research areas of the discipline.
2	NeuGaze: A biomarker based, easy-to-use, language agnostic, Computer-based Screening Battery for Cognitive Health	PI - Uttama Lahiri Co-PI Manasi Kanetkar	This will involve use of a computer-based cognitive test battery along with quantification of one's cognitive health in terms of gaze indices and brain signal based indices	
3	Design and development of wearable sensors for monitoring human physiology and movement.	PI: Biswajit Saha Co-PI: Uttama Lahiri	The selected candidate for this project will work on synthesizing advanced/nanomaterial, characterizing materials, patterning sensing elements, and designing sensors. After the sensor developmental work, the candidate will closely work with the research group of sensor data analysis and monitoring groups.	
4	Wearable robotic exoskeleton for human movement restoration - design, control, and experimentation	PI- Vineet Vasistha	Exoskeletons are robotic systems that are used in parallel with human body segments for assisting disabled individuals. In our lab, we are developing wearable robotic exoskeletons that are light-weight, flexible, and can be worn on legs, arms, or trunk. This project will involve activities including design and development, control, and testing to apply controlled external forces during various activities of daily living, such as walking, lifting weight, drawing, etc.	
5	Techniques for movement characterization and	PI- Vineet Vasistha	We propose to develop a portable sensor system that serves as a diagnostic tool for movement	

	performance measurement using portable sensor system		measurement and correction. The system will comprise a well-established integrated network of microcontrollers and sensors. The aim is to develop techniques, such as a deep learning solution, to recognize human activity and characterize the movement parameters. It is proposed to develop an android/web based application to use the information for sports and rehabilitation applications, such as athletic performance during a sports activity or patient movement recovery.	
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Theme: Space Research

Coordinator: Prof. Joycee Mekie

Space Research group pursues themes that are deeply integrated with modern facets of space exploration encompassing electronics, telecommunications and materials.

Sl. No.	Project Title	Investigators	Project Description	Minimum Eligibility Requirements
1	Radiation Hardened Systems for Space Applications:	PI- Joycee Mekie Co-PI- Sameer Kulkarni	Electronics used in Space Applications are designed differently to ensure error-free operations and are becoming increasingly relevant considering a broader reach of space research. Soft-errors in space electronics are caused due to the radiations from solar flares impacting the systems. In this project new methodologies and approaches to build electronic systems suitable for space applications will be explored, including processors, memory, serial interface protocols, etc.	First Class or 65% marks (60% for SC/ST/PD) or 6.5(6.0 for SC/ST/PD) CPI/CGPA on the scale of 10 in: BE/BTech/ME/MTech or Equivalent degree in the broad area of Electrical and/or Electronics engineering or Computer Science and/or Engineering, OR BE/BTech/ME/MTech or Equivalent degree in other branches of Engineering may be considered in areas consistent with the broad area of MicroElectronics and VLSI. Preference will be given to candidates having experience relevant to the project domain.

Theme: Data Science for Earth Science

Coordinator: Prof. Udit Bhatia

Earth and environmental sciences are relying heavily on collection and scrutiny of real data. The interplay between data and earth science provides critical inputs for large scale processes.

Sl. No.	Project Title	Investigators	Project Description	Minimum Eligibility Requirements
1	Application of data science to study morphological (physical) studies of rivers at global scale;	PI- Vikrant Jain and Udit Bhatia	Projects will develop algorithms for auto- extraction of physical features from digital data (DEM and satellite data) at global scale and involve analysis of large data sets representing different types of climate and landscapes. For example, data interpretation will aspire to understand (i) Fundamental nature of river processes and its controls, (ii) Temporal variability in river processes at decadal time scale	MSc in any subject of Sciences with 65% marks (60% for SC/ST/PD) or a CPI/CGPA of 6.5 (6.0 for SC/ST/PD) out of 10 of BTech in Computer Science, Electrical Engineering, Geomatics, Hydrology, Civil Engineering or related subjects with 65% marks (60% for SC/ST/PD) / CPI/CGPA of 6.5 (6.0 for SC/ST/PD) out of 10. Desirable - (1) CSIR-NET, INSPIRE fellowship or GATE qualified, (2) Good command on computing.
2	AI driven 3D Mapping of Ocean Bed; Shanmuganathan Raman and Pankaj Khanna (PI)	PI- Shanmuganathan Raman and Pankaj Khanna		

Theme: Electric Vehicles

Coordinator: Prof. Ragavan K

Electric vehicles are at the forefront of efforts to address sustainability in transport. Projects in this theme will address specialized aspects of electric vehicle design and operation.

Sl. No.	Project Title	Investigators	Project Description	Minimum Eligibility Requirements
1	Improving range of Electric Vehicle by deploying regenerative braking	PI: Ragavan K. , Naran Pindoriya and Soumyadip Sett (co-PI)	While braking, a part of the kinetic energy associated can be converted to electrical energy and stored in the battery. With this, the range of the vehicle improves.	BE/BTech and/or ME/MTech in the area of Electrical engineering OR in other branches consistent with the mentioned research areas. CPI/CGPA: 6.5 (6.0 for SC/ST/PD) CPI/CGPA on the scale of 10

Theme: Energy

Coordinator: Prof. Naran Pindoriya

Sustainable solutions to meet growing energy demands of the planet forms one of the single biggest challenges for humanity. Projects in this theme address fundamental and applied aspects of addressing these challenges.

Sl. No.	Project Title	Investigators	Project Description	Minimum Eligibility Requirements
1	Robust control for minimizing electrical power fluctuations in wind energy conversion system with the aid of battery storage:	Ragavan K (PI), Naran Pindoriya and Jaichander Swaminathan (co-PI)	As wind is of intermittent nature, the electrical power generated is not stable. To minimize the fluctuations, battery energy storage can be adopted. This requires an efficient and robust control of the power drawn from the battery.	BE/BTech and/or ME/MTech in the area of Electrical engineering OR in other branches consistent with the mentioned research areas. CPI/CGPA: 6.5 (6.0 for SC/ST/PD) CPI/CGPA on the scale of 10.CPI/CGPA: 6.5 (6.0 for SC/ST/PD) CPI/CGPA on the scale of 10

Theme: Food & Agricultural Technology

Coordinator: Prof. Subramanian Sankaranaryanan

Decades after green and white revolutions, the country faces a new set of challenges to meet ever growing demands of food. Projects in this theme are aligned with fundamental concepts and applications that are ultimately expected to address these challenges.

Sl. No.	Project Title	Investigators	Project Description	Minimum Eligibility Requirements
1	Enhancing agricultural productivity using the Green synthesis of nanoparticles	Jhuma Saha and Subramanian S (co-PI)	Synthesis of nanoparticles/quantum dots (QDs) using the green chemistry approach. The objective is to utilize the prepared QDs to cure plant diseases and to enhance agricultural productivity.	MSc in chemistry/MSc or M.Tech in material science/MSc or M.Tech in Biotechnology with at least 60% (or CPI 6.0).

Theme: Computational Sciences & Engineering

Coordinator: Prof. Kaustubh Rane

At IIT Gandhinagar, we have several research groups working on various aspects of theory and computation. Leveraging High Performance Computing (HPC) facilities that enable large-scale simulations, researchers from diverse disciplines such as Chemistry, Biological, Chemical, Mechanical, and Materials Engineering are in the pursuit of some of the most challenging focus areas such as design and development of novel materials, modeling molecular forces, biomolecular simulations, drug discovery, fluid-particle interactions, energy storage devices, advanced manufacturing etc.

Sl. No.	Project Title	Investigators	Project Description	Minimum Eligibility Requirements
1	Machine Learning Potentials for Atomistic Modeling of Materials.	Anirban Mondal (PI)	This project aims to address the trade-off between accuracy and speed that can be solved by interatomic potentials developed by employing machine learning techniques. These potentials aim to provide the accuracy of electronic structure calculations at approximately the computational cost of force fields. This project seeks to build such machine-learning potential to perform material and reaction simulations which typically deal with slow chemical bond evolution in complex environments.	B.E./B.Tech./M.Sc. (graduated or in the final semester) with a qualified NET/GATE score M.E./M.Tech. (graduated or in the final semester) At least 65% marks or 6.5 CPI marks in M.Sc./B.Tech./M.Tech./BS (IISc, IISER)/BS-MS (IISER) or equivalent degree
2	High Throughput Computational Screening of Organic Semiconductors:	Anirban Mondal (PI)	A systematic approach that links chemical structure to macroscopic properties would be incredibly beneficial to optimize the design of organic electronic devices. Exploring and screening a chemical space using high-throughput computing provides an efficient route to explore a diverse set of candidate structures by understanding the structure-property relationship. The idea here is to employ a machine-learning framework to screen potential organic compounds to improve the overall performance of organic photovoltaic devices.	

3	Computation of Thermodynamic and Transport Properties of Energetic Materials using Molecular Scale Simulations:	Dilip Sundaram (PI)	Energetic materials find applications in propulsion systems and explosives in view of their high energy density. The project aims to quantify the thermodynamic properties (such as free energies, melting points etc.) and transport properties (thermal conductivity, heat transfer coefficients etc.) of novel metal-based energetic materials using both molecular dynamics and monte-carlo simulations.	
4	Modeling and Simulation of Combustion and Propulsive Performances of Metal-Based Propellants	Dilip Sundaram (PI)	Energetic materials find applications in propulsion systems and explosives in view of their high energy density. The project aims at developing a comprehensive model of combustion of novel metal-based propellants. An array of physicochemical processes such as heat transfer, fluid mechanics, high pressure thermodynamics and transport, chemical reactions will be modeled. The goal is to predict the combustion rates as well as propulsive performances of these propellants.	
5	Using theory and molecular simulations to study the adsorption of small molecules on tethered polymers.	Kaustubh Rane (PI)	Polymers tethered to nanoparticles or surfaces are finding several applications. We want to explore their use as “smart” adsorbents. The “smartness” refers to the ability of polymers to respond to the process conditions in a beneficial way. The aim is to rationally design such polymers using molecular simulations and theory.	
6	Developing theoretical and computational methods to study density fluctuations near solid-	Kaustubh Rane (PI)	The liquid-vapor interface , and the interface between hydrophobic solid surface and water are characterized by enhanced density fluctuations.	

	liquid and liquid-vapor interfaces.		The above fluctuations have potential applications in micro and nanofluidic devices. Computational studies have been a challenge due to limitations of present methods. We aim to develop new computational tools to study such fluctuations with greater precision.	
7	Molecular Dynamics simulations of the Nuclear Pore Complex (NPC)	Mithun Radhakrishna (PI)	. The NPC is made of intrinsically disordered peptides known as FG NUPs that act as molecular sieve regulating transport in and out of the nucleus.. The project would involve carrying out all atom and coarse grained molecular dynamics simulation to understand the mechanism of transport through the NPC.	
8	Identification of Aggregation Prone Regions using ML based algorithms.	Mithun Radhakrishna (PI)	Protein aggregation is known to be the main cause for many neurodegenerative diseases like Alzheimer's and Parkinson's diseases. This project would involve a combination of simulations and machine learning to develop algorithms that can effectively identify the aggregation prone regions in proteins.	
9	Molecular Dynamics Simulations of Polymer Grafted Nanoparticles for applications in batteries and supercapacitors.	Mithun Radhakrishna (PI)	Addition of grafted nanoparticles has found many applications in the field of material design, drug delivery and energy storage. By controlling the assembly of NPs, one can effectively tune the optical, mechanical, chemical and electrical properties. The project involves studying the effect of grafted NPs on ion transport for application in batteries and supercapacitors.	

10	Development of Machine-learning based force fields for multi-component metallic alloys.	Raghavan Ranganathan (PI)	<p>Multi-component alloys such as high-entropy alloys have ushered a new paradigm in materials design with fascinating applications. The multi-body interactions/correlations in such systems are poorly understood. This project aims to develop accurate and high-fidelity force fields to describe various alloy systems, incorporating first-principles (DFT) simulations and machine learning algorithms.</p>	
11	Atomistic simulations of materials under extreme conditions:	Raghavan Ranganathan (PI)	<p>Materials subject to extreme conditions such as high strain rate deformation (e.g. shock loading, ballistic impact, etc.) and high pressures/temperatures (e.g. pyrolysis/ablation/combustion) are inherently difficult to model, but are crucial for cutting edge, high-tech applications. This project will involve multi-scale simulations of such extreme scale deformation using techniques such as molecular dynamics, finite element methods and machine learning.</p>	
12	Development of crystal plasticity based frameworks (theory and computation) to study fracture behavior in high entropy alloys.	Ravi Ayyagiri (PI)	<p>High entropy alloys present enhanced fracture toughness characteristics even at low temperatures. We investigate the mechanisms of void growth and coalescence that drive failure in these materials through development of physics based continuum models that account for response in individual grains.</p>	
13	Computational study of mechanical behavior in sponge like materials	Ravi Ayyagiri (PI)	<p>Inspired by natural selection, the project focuses on understanding the role of hierarchies in materials that exhibit high energy absorption characteristics. The goal is to decrypt the choice of order of hierarchy and its relation to property-performance aspects.</p>	

			The study includes both theoretical and computational investigations ranging over several orders of hierarchy.	
14	Computational Ayurvedic Drug Discovery.	Sairam Mallajosyula (PI)	The project focuses on the development of force fields for describing ayurvedic phytochemicals. An accurate force field would enable studying the interaction of these phytochemicals with target proteins.	
15	Computational investigations of graphene nanopores and nanoslits for biomolecular detection:	Sairam Mallajosyula (PI)	Graphene presents itself as an excellent 2D system for applications in membrane and separation technologies. Our recent developments on polarizable graphene allow us to study the polarization dynamics at the graphene interface.	
16	Network modeling of biological systems	Ashutosh Srivastava (PI)	Networks provide an excellent framework for modeling real world systems with interacting elements. The network formalism has been used successfully to model biological systems at various scales, from molecular interactions to interactions of species in an ecosystem. In this project, we will be modeling the interactions between proteins as networks by taking cues from their structure. A background in graph theory, programming and/or structural biology will enable the students to apply these concepts in developing network based models of protein-protein interactions.	
17	Integrative modeling and molecular dynamics simulations of biological	Ashutosh Srivastava (PI)	Most of the cellular functions are carried out by biological macromolecules by forming	

	macromolecular complexes		<p>stable or transient complexes. Understanding the structure and dynamics of these macromolecular complexes has been challenging using any single experimental technique. In this project, we will use integrative modeling methods, that involves integrating structural data from several experiments at multiple spatial and temporal resolution, to study the structure and dynamics of these macromolecular complexes. A particular focus of the project is on the macromolecular complexes involved in circadian regulation.</p>	
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Theme: Sustainability Coordinator: Prof. Aashish Xaxa				
Sl. No.	Project Title	Investigators	Project Description	Minimum Eligibility Requirements
1	Sustainable Development in Tribal Areas of India.	Aashish Xaxa	<p>Development is often marked by dispossession of people from their land and resources, accentuating poverty, health hazards, causing damage to the ecology and environment, and livelihood, combined with the</p>	1. M.A./MSc in any subject of Humanities/Social Sciences/Sciences with 60% marks (55% for SC/ST/PD) or a CPI/CGPA of 6.0 (5.5 for SC/ST/PD) out of 10

			<p>absence of share and participation in development. Keeping these contexts in mind, this project would examine the challenges of inclusive and sustainable urban development in tribal areas of India.</p>	<p>2. Desirable: NET/CSIR, INSPIRE Fellowship or GATE qualified.</p>
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