Birla Institute of Technology and Science, Pilani, Pilani Campus
Department of Chemical Engineering
Ph.D. Research Topics
First Semester 2023-24

Supervisor: Dr. Mohit Garg

Project Topic: Computational modeling of nanomaterials and biomaterials for energy and environmental applications

Broad Research Area: Computational material science, Polymer physics and chemistry, Biomolecular modeling

Background of Research: The computational modeling has now become an important tool not only understand the materials properties but also to design and develop new materials. The proposed study will be based on multiscale modeling of various polymers and biomaterials to be used in organic electronics and organic bioelectronics applications. The focus will be on understanding the electronic, morphological and mechanical properties of these materials. The modeling work will include Quantum Mechanical calculations, Molecular Dynamics (MD) simulations and Monte Carlo (MC) simulations. Another aspect of the modeling will be understand the properties of the materials at different length scales and time scales. So, the development of coarse grained models for different materials will also be an integral part of the proposed work.

Requirements:

- Experience or willing to learn Density functional theory and MD/MC simulations.
- Knowledge or willing to learn programming language, e.g., MATLAB, python, C/C++.
- Self-motivated, keen to learn new simulation methods, and ability to solve problems independently.
- Good proficiency in technical writing.

Publications

- Mohit Garg and Venkat Padmanabhan, ***Scientific Reports*** 6, 33219, 2016.
- Nicolas Rolland, Aleksandar Mehandzhiyski, Mohit Garg, Mathieu Linares, and Igor Zozoulenko, ***Journal of Chemical Theory and Computation***, 16 (6), 3699–3711, 2021.
- Mohit Garg, Mathieu Linares, and Igor Zozoulenko, ***Biomacromolecules***, 21 (8), 3069–3080, 2020.

Please refer to my google scholar
https://scholar.google.co.in/citations?user=w2l3zU0AAAAJ&hl=en

Essential Qualifications:

- M.E./M.Tech. with at least 60% marks in Chemical/Mechanical/Materials/ Nanotechnology/Biotechnology.
- M.Sc. with at least 60% marks in Chemistry/Materials Science/Nanotechnology/ Physics/Mathematics.

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Supervisor: Dr. Hare Krishna Mohanta

Topic: Development of Machine Learning and Molecular Simulations Driven Smart Gas Sensors for Toxic Gases

Brief Description of the topic:

There are several pollutant gases that are harmful to human beings and need to be detected. The high-performance sensing materials to be used in gas detection will be identified using molecular simulations, including molecular dynamics simulations and grand canonical Monte Carlo simulations. Machine learning techniques will be used to develop smart gas sensors. Molecular simulations and machine learning techniques together will help to design highly selective and sensitive smart gas sensors to be operated at room temperature.

Essential Minimum Qualification:

The candidate must be a graduate/post graduate in Chemical Engineering or allied disciplines or MSc in Physics/Chemistry/Material Sciences/Nanotechnology with at least 60% marks.

Desired Qualification:

Knowledge of programming languages like MATLAB, python, C/C++ will be helpful but not essential. Candidates should be willing to learn new modeling and simulation methods or computational skills.

Selected Publications:

1. Venkata Vijayan S., **Hare K. Mohanta**, Ajaya Kumar Pani (2022). Adaptive non-linear soft sensor for quality monitoring in refineries using Just-in-Time Learning—Generalized regression neural network approach, Applied Soft Computing, 119, 108546, ISSN 1568-4946. IF:8.26. *Link*

2. Venkata Vijayan S, **Hare Krishna Mohanta**, Ajaya Kumar Pani, (2021), Support vector regression modeling in recursive just-in-time learning framework for adaptive soft sensing of naphtha boiling point in crude distillation unit, Petroleum Science, 18 (4), 1230-1239, ISSN 1995-8226. IF: 4.76. *Link*
3. Singh, H., Pani, A. K., **Mohanta, H. K.** (2019). Quality monitoring in petroleum refinery with regression neural network: Improving prediction accuracy with appropriate design of training set. Measurement, 134, 698-709.
4. Pani, A. K., Amin, K. G., & **Mohanta, H. K** (2016), "Soft sensing of product quality in the debutanizer column with principal component analysis and feed-forward artificial neural network", Alexandria Engineering Journal, 55, 1667-1674.Pani, A. K., **Mohanta, H. K** (2016)," Online monitoring of cement clinker quality using multivariate statistics and Takagi-Sugeno fuzzy-inference technique", Control Engineering Practice, 57, 1-17.
5. Pani, A. K., & **Mohanta, H. K.** (2015). Online monitoring and control of particle size in the grinding process using least square support vector regression and resilient back propagation neural network. *ISA transactions*, *56*, 206-221. *Link*
6. Pani, A. K., & **Mohanta, H. K.** (2014). Soft sensing of particle size in a grinding process: Application of support vector regression, fuzzy inference and adaptive neuro fuzzy inference techniques for online monitoring of cement fineness. *Powder Technology*, *264*, 484-497. *Link*
7. Pani, A. K., Vadlamudi, V. K., & **Mohanta, H. K.** (2013). Development and comparison of neural network based soft sensors for online estimation of cement clinker quality. *ISA transactions*, *52*(1), 19-29. *Link*

For more details, contact:

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Supervisor: Dr. Banasri Roy

Title of the project: Conversion of Agricultural Residues to Value added materials (catalysts, adsorbent, etc.) and their applications.

Project Description: Driven by the necessity of utilizing unexplored but abandoned renewable agricultural residues and developing technology to enhance renewable energy resource production, this project proposal was undertaken with the following major objectives:

- To develop methods for maximizing the conversion of locally (in India) available crop-based residual biomass to high surface area, high porosity, and controllable pore size (mesoporus range) activated carbon (AC) and graphene oxide (GO), and etc., of functionality related to applications. Both thermo-chemical and hydrothermal processes will be explored.
- To examine relevant physicochemical properties of carbonaceous materials.
- To study catalytic and other activity of the carbonaceous materials.
- Correlate activity of the carbonaceous materials with the corresponding physicochemical properties for further optimization of the preparation conditions of materials with the aim of maximizing the catalytic activity, stability, and recyclability of the carbonaceous materials.

The scope will be to explore different possible modifications and/or new designs that can be applied on the carbonaceous materials from agricultural residues and their applications in order to understand and manipulate the process mechanisms.

Publications of the Supervisor: Pls visit
https://scholar.google.com/citations?hl=en&user=HF4Inh8AAAAJ&view_op=list_works&sortby=pubdate
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Supervisor: Dr. Krishna C. Etika

Project Topic: 3-D Printed Hybrid Polymer Nanocomposites for Stealth Applications

Broad Research Area: Advanced Materials, Nanotechnology, Polymer Nanocomposites

Background of Research: Fused deposition modeling (FDM) is a heat-assisted 3D printing process in which the molten polymer is extruded out of a nozzle, deposited onto a substrate, cooled down, and solidified. FDM generates multilayered, multifunctional structures as well as patterned structures with complex geometries. The multilayered patterned structure is a novel empowering technology that allows controlling the properties of each layer/section of the shield and thus manipulating the shielding mechanisms, not possible in common molding techniques. Another significant advantage of 3D printing is the development of stealth shields with complex geometries, which is a critical need in advanced industries such as aerospace and defense. The technology of the 3D printed shields is in its infancy and the underlying science is an ongoing subject of investigation in the literature. To explore the realm of 3D printed shields we will employ a variety of strategically chosen conductive, magnetic, and dielectric nanofillers. The ultimate outcome of this research would be to produce fully biodegradable, mechanically robust, lightweight materials with greater than 20 dB microwave absorption loss.

Responsibilities/Expected Outcome from the student:
This project involves the 3D printing of pristine polymer and its nanocomposites to create radar-absorbing materials with complex geometries. We will investigate the influence of different parameters, such as filler loading, the electrical conductivity of the filament feedstock, number of layers, the architecture of the scaffold, patterned structure, and dispersion state of filler, on the final electrical, mechanical, and shielding properties of 3D printed samples. The primary objectives of the proposed research expected from the student are as follows:

1. **Task 1**: We will use the chemical technique to synthesize magnetic and dielectric nanoparticles of interest. The nanoparticles would be carefully selected based on their properties.
2. **Task 2**: We will develop and characterize biodegradable (Polylactic acid-based) nanocomposite pellets and filaments by mixing various types of nanofillers from Task 1. The mixing will be performed at various loadings of nanofillers ranging from 0.1-5.0 wt%.
3. **Task 3:** We will compression mold the materials into various shapes and characterize them. The compression-molded samples will be used as a benchmark to evaluate the quality of nanofillers employed and the performance of the 3D printed samples.
4. **Task 4:** We will 3D print the developed pristine polymer filaments using the FDM technique and characterize the samples.
5. **Task 5:** We will 3D print the developed nanocomposite filaments using the FDM technique and characterize the samples.

Publications
https://scholar.google.com/citations?user=e4kYT2IAAAAJ&hl=en

Essential Qualifications:
- M.E./M.Tech. with at least 60% marks in Chemical/Materials/Nanotechnology
- M.Sc. Chemistry/Materials Science/Nanotechnology/Physics candidates with a very good track record will also be considered

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Supervisor: Dr. P C Sande

Project Topics which many be taken independently or combined suitably: (a) Visualization and simulation of multiphase-flow (b) CFD simulation of multiphase flow

Broad Research Area: multiphase flow (gas-particle flow hydrodynamics)

Background of Research:

(a) PIV is a non-intrusive technique to monitor and measure dynamic flow parameters. It provides insights into both quantitative and qualitative aspects of flow. PIV can be used to find velocity vector fields for all kinds of flows, be it for all types of fluidization in reactors or even flow gas-solid flow in human anatomy.
(b) The field of computational science is widely used in design, scale-up and improvement of industrial chemical engineering unit-operations. Fluidized beds in particular are widely employed, and are among the more complex unit operations owing to the variety of regimes that they display, such as: Homogeneous, bubbling, turbulent and slugging fluidization. These regimes emphatically affect reactor performance. They are ideal to be investigated by computational and simulation tools that have developed over the past decade such as: ANSYS Fluent, OpenFOAM, COSMOL etc. Machine Learning can be integrated into the procedure to derive in depth analysis.

Preferred skills:

1. Experimental skills preferably in using high-sensitivity equipment
2. Knowledge of basic fluid dynamics
3. Adequate scientific writing skills
4. Visual discernment of patterns/ pattern recognition
5. Basic programming experience, such as in Matlab/ C++/ Python, Preferred experience with CFD software such as ANSYS ans COMSOL

Publications

- Ajita Neogi, Hare K. Mohanta, Priya C. Sande, Particle image velocimetry investigations on multiphase flow in fluidized beds: A review, Flow Measurement and Instrumentation, Volume 89, 2023,102309,ISSN 0955-5986
- P.C. Sande, S. Ray, Fine Mesh Computational Fluid Dynamics Study on Gas-Fluidization of Geldart A Particles: Homogeneous to Bubbling Bed, Industrial & Engineering Chemistry Research, 55 (2016) 2623-2633.
- P.C. Sande, S. Ray, Mesh size effect on CFD simulation of gas-fluidized Geldart A particles, Powder Technology, 264 (2014) 43-53.

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Supervisor: Prof Suresh Gupta

Project title: Development of Eco-friendly microporous polymer-metal frameworks for pollutant adsorption

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