P Surya Samyog

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EDUCATION

National Institute of Technology Calicut **2021 – 2025**
Bachelor of Technology in Materials Science and Engineering - ***CGPA: 8.64 (GPA: 3.5)*** *Kozhikode, Kerala*

- ***Relevant Modules****: Computational Methods for Materials Science, Neural Networks for CFD, Machine Learning for Data Science and Analytics, Structure of Materials, Physics and Chemistry of Materials, Computer Programming, Thermodynamics, Energy Materials and Technology, Mathematics (I - IV)*

Central Board of Education **2020 – 2021**
12th Grade - ***Percentage: 95.2*** *Alappuzha, Kerala*

Central Board of Education **2018 – 2019**
10th Grade - ***Percentage: 97.6*** *Alappuzha, Kerala*

RESEARCH EXPERIENCE

Computational Nanotechnology Laboratory **Aug 2024 – May 2025**
Undergraduate Researcher *MSED, NIT Calicut*

- Worked extensively on DFT calculations using Quantum ESPRESSO (QE), gaining strong proficiency in quantum chemical simulations and writing QE input files.
- Hands-on experience with High Performance Computing environments and Bash scripting for executing DFT calculations.
- Developed Python scripts to automate DFT workflows and generate DFT dataset. Edited source codes of simulation packages for custom calculations and to meet system requirements.
- Provided guidance and support to peers in the lab on using QE.

PROJECTS

Enhancement of HER performance of 2D ReS_2 via Bimetallic Nanoclusters: A Machine Learning-Assisted DFT Study | *Quantum Espresso, DScribe, Cluskit, BURAI 1.3* **Jan 2025 - Present**

- Investigating the electrocatalytic properties of pure rhenium sulfide monolayer using DFT simulations.
- Conducted in-depth study of its electronic structure using Quantum Espresso and VESTA. Studied the catalytic activity of the basal plane by calculating the hydrogen adsorption energy.
- Developing a database of bimetallic transition metal nanoclusters (13 atoms, Icosahedral geometry) with identified adsorption sites and optimised structures using DFT and Cluskit, followed by calculation of their hydrogen adsorption energies and feature space engineering to train a predictive ML model for high-throughput screening of metal nanoclusters.

Equivariant Graph Neural Networks with Higher-Order Node Interactions **May 2025 - Present**
PyTorch, PyTorch Geometric

- Implemented an EGNN model from scratch using PyTorch and PyTorch Geometric based on existing research to study molecular property prediction.
- Used the QM9 dataset to validate the model's ability to capture geometric symmetries and equivariant transformations.
- Currently conducting a literature review and formulating the mathematical foundations to incorporate angular information (3-node) into the EGNN framework as a foundational step toward enabling higher-order node interactions.

DFT-Driven Generation of ANN Potentials for 316LN SS using ænet **Aug - Dec 2024**
Quantum Espresso, ænet, ASE, BURAI 1.3

- Developed a Python-based workflow to automate DFT dataset generation, including introducing defects, strain, and perturbations using Atomic Simulation Environment (ASE).

- The ænet package is used to develop an HDNNP model to generate ANN potentials.

Physics-Informed Neural Networks for Solving Nonlinear PDEs using DeepXde **March 2025**

DeepXde, Python, Tensorflow, Matplotlib, Numpy

- Implemented inverse PINNs to solve the Navier-Stokes equations by identifying unknown flow parameters from time-resolved 2D velocity and pressure field data of fluid flow past a cylinder.
- Modelled and visualised phase separation dynamics using the Allen-Cahn equation; extracted and analysed contour plots for system evolution.
- Simulated single soliton wave propagation by solving the Korteweg–de Vries (KdV) equation using PINNs.

Study of Mechanical Properties and Microstructure of Copper based Musical Instrument Strings | *Tensile & Hardness Testing, Polishing, Optical Microscopy, SEM* **Jan - May 2024**

- Cross-sections of copper-based musical strings with different elemental compositions were polished and then etched. The etched samples were examined under an optical microscope to classify the grain structure, providing insights into their mechanical properties.
- Uni-axial tensile tests and micro-hardness tests were conducted on the strings. The results were analysed to compare the effects of different elemental compositions on strength, ductility, and hardness.
- SEM images were taken for all samples, including polished, etched, and mechanically tested ones, to examine surface morphology and microstructural features. EDS analysis was performed to determine the actual elemental composition and assess variations from the intended alloying elements.

ADDITIONAL EXPERIENCE

ZFWPC – ZF Friedrichshafen AG **May 2024 – July 2024**

Data Analysis and Process Engineering Intern *Coimbatore, Tamil Nadu*

- Conducted research on lean management and production process flow and constructed a current state VS mapping to identify inefficiencies, reduce lead time, and minimise waste.
- Developed DAX measures to analyse large datasets, enabling real-time inventory tracking, efficient material ordering and classify axle parts by model to track available inventory.

CONFERENCES AND RESEARCH VISITS

MEEHCON'24 **December 2024**

International Conference on Materials for Energy, Environment & Healthcare *NIT Calicut*

- Presented a research poster titled **DFT-driven Generation of ANN Potentials for 316LN Stainless Steel** at MEEHCON'24, showcasing my work in computational materials science. Engaged with esteemed professors, attended thought-provoking sessions, and networked with researchers from diverse disciplines and global institutions.

Summer Research Programme at City University, Hong Kong **July 2025**

School of Energy and Environment *CityU, HKG*

- Conducted a thorough literature review and collaborated closely with the research group to develop a research proposal titled **Lifelong Machine Learning Potentials for Complex 2D-TMD Aqueous Systems Using EGNNs**. The idea was developed from scratch, and a detailed methodology was outlined for the proposed project.

CERTIFICATIONS AND ADDITIONAL COURSES

DFT Modelling of Advanced Materials (Hands-on-Training) **March 2025**

Centre for Advanced Computational Research *New Delhi*

IBM AI Engineering Professional Certificate **Present**

Coursera *Online*

Basic Numerical Methods **Present**

TU Dresden *Online*

LEADERSHIP / EXTRACURRICULAR

The Literary and Debating Club **Oct 2023 – Oct 2024**
General Secretary *NIT Calicut*

- Led initiatives on mental health and Pride, revived *Kaapikootam* open house discussions, organised cultural and literary events, laid the groundwork for Sahiti literature fest, and fostered a collaborative club environment.

Kerala Literature Fest 2024 **January 2024**
Volunteer *Kozhikode*

- Volunteered at Asia's largest literature festival, leading a team of volunteers and ensuring smooth guest–volunteer communication while addressing guest needs.

Tathva 2023 **Aug 2023 – Jan 2024**
Design Team Head *NIT Calicut*

- Led a team of graphic designers, creating social media posters for the fest and fostering a collaborative environment to ensure timely delivery.

Miraqui – Fashion Show Team **April 2023 – Oct 2024**
Captain and Marketing Head *NIT Calicut*

- Coordinated a large team to ensure smooth collaboration, organised model practice sessions, and managed team finances, including preparing the annual budget.

CREATIVE WORK

The Brand Project - Freelance **June 2023**
Brand Designer *Remote*

- Provide freelance brand solutions by designing logos and brand identities for various firms, events, and clients. Collaborated with multiple clients to align visual identity with brand vision, including a recent project where I co-developed complete branding and a website for a client.

The Literary and Debating Club **Sep 2022 – Oct 2024**
Graphic Designer & Illustrator *NIT Calicut*

- Designed cover posters that visually captured the essence of peer-written articles, and created promotional materials for events, debates, and talk sessions, helping shape the club's visual identity.

KNOWN LANGUAGES

- English
- Malayalam
- Hindi
- Tamil

End