Rudra Patel

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OBJECTIVE

Motivated undergraduate student in Materials Engineering with a strong interest in computational materials science, machine learning, and materials informatics. Passionate about solving complex materials challenges through data-driven and physics-informed approaches, and contributing to impactful research and innovation in materials discovery and design.

EDUCATION

- **Indian Institute of Technology, Jodhpur**   CGPA: 7.7/10   Jodhpur, India
  Bachelor of Technology - Materials Engineering (Specialization: Computational Materials) August 2022 – June 2026

PUBLICATIONS

- **Rudra Patel** et al. *Uncertainty-Aware Prediction of Mechanical Properties in Graphene Using Random Forest and Monte Carlo Simulations.* Under Review *meccanica*, 2025.

- **Rudra Patel** et al. *In-situ Monitoring and Dimensional Analysis of Additive Manufacturing Using Deep Learning and 3D Reconstruction.* (Manuscript prepared for submission)

- **Rudra Patel** et al. *Real-Time Automated Layer Identification of 2D Materials: A Practical Deep Learning Framework for High-Throughput Characterization.* (Manuscript prepared for submission)

EXPERIENCE

Materials Informatics Intern - Ai Materia, Toronto, Canada (Remote)
Materials Informatics Intern   *July 2025 – Present*

- **Dataset Engineering for Metals and Alloys**: Designing robust methodologies to curate clean, reliable, and high-quality datasets from diverse sources focused on metallic systems and alloys.

- **Addressing Data Scarcity in Materials Informatics**: Tackling the core challenge of limited high-quality data in materials science by developing scalable workflows for data collection, preprocessing, and integration.

- **Use Case Exploration**: Exploring practical applications of curated datasets in predictive modeling, property estimation, and design of novel metallic materials.

Research Intern - Xi'an Jiaotong-Liverpool University, China
Materials Informatics Research Intern   *June 2025 – Present*

- **ML-Based Property Prediction of Li-based Oxides**: Investigated bandgap and formation energy trends in layered lithium transition metal oxides using data-driven approaches.

- **Dataset Creation and Feature Engineering**: Curated a dataset using Materials Project API; applied matminer for materials featurization and performed data cleaning.

- **Feature Selection and Model Interpretability**: Utilized Gradient Boosted Decision Trees (GBDT) for identifying important features; trained multiple predictive models and performed comparative analysis. Applied SHAP and symbolic regression techniques to ensure model transparency and interpretability.

Research Intern - Indian Institute of Technology Bombay, India
Computational Materials Research Intern   *May 2025 – July 2025*

- **Anisotropic Behavior Simulation of AM SS201 Steel**: Simulated the anisotropic mechanical response of additively manufactured SS201 steel using the DAMASK framework and 2D EBSD data.

- **3D RVE Generation and Simulation Setup**: Constructed an accurate 3D representative volume element (RVE) from 2D EBSD data; prepared input scripts and performed simulations on high-performance computing clusters.

- **Parameter Fitting and Result Analysis**: Carried out high-throughput simulations for parameter fitting and conducted detailed visualization and analysis of stress-strain response and texture evolution.

Research Intern - Huazhong University of Science and Technology (HUST) ,China
Computational Materials Research intern   *Jan 2025 - May 2025*

- **Uncertainty-Aware Mechanical Property Prediction**: Developed a machine learning model integrated with Monte Carlo simulations to predict mechanical properties of 2D materials with uncertainty quantification.

- **Data-Driven Materials Modeling**: Utilized machine learning techniques to analyze and predict material behavior, enabling faster and cost-effective alternatives to traditional molecular dynamics simulations.

ONGOING RESEARCH PROJECTS

- **ML-Based Property Prediction of Li-based Oxides**: Used data-driven techniques to predict bandgap and formation energy of layered lithium transition metal oxides with interpretable ML models and feature analysis.

Rolling-Based Study of Ti-5553 Alloy (Materials Processing and Characterization) *(Aug'24 – May'25)*
Dr. Jaiveer Singh

- Synthesized and processed the Ti-5553 alloy through alloy preparation, rolling, and mechanical testing workflows.
- Performed sample grinding, polishing, etching, and hardness testing to study the mechanical response.
- Captured microstructural images using microscopy techniques to analyze grain size and microstructural evolution.
- Investigated the effect of rolling on hardness variation and phase transformations in the alloy.

Machine Learning-Driven Image Processing of Electron Micrographs *(Aug'23 - Dec'23)*
Design Credit Project, Mentor: Prof. Devendra Singh Negi, **GitHub**

- Led a comprehensive project focused on TEM (Transmission Electron Micrograph) data analysis.
- Developed a versatile solution to extract and process information from diverse file formats such as .txt, jpg, and hdf5.
- Employed 2D interpolation techniques to enhance image quality and meticulously scanned each pixel to capture critical data.
- Utilized image kernels for efficient image processing, generating multiple datasets, and applied machine learning tools to further refine and analyze the processed images.

Bulk Modulus Calculation of Si and Ni using Quantum ESPRESSO *(June'24)*
Prof. Appala Naidu Gandi

- Executed precise structure optimization and energy computations for Si and Ni.
- Identified equilibrium lattice constants and performed fourth-degree polynomial fitting.
- Derived bulk modulus through curvature analysis at equilibrium lattice points.

Electronic Band Structure and Density of States Analysis using Quantum ESPRESSO *(July'24)*
Prof. Appala Naidu Gandi

- Conducted self-consistent and non-self-consistent field calculations for Si and Al.
- Computed and plotted Density of States (DOS).
- Analyzed electronic band structure along k-paths.
- Determined and compared bandgaps with literature values.
- Investigated and reported discrepancies between calculated and experimental bandgaps.

Material Stability Prediction using Machine Learning and Neural Networks *(Jan'24 - Mar'24)*
Self Project, ⍥ **Github**

- Developed a material stability prediction model using various machine learning algorithms and neural network architectures.
- Conducted extensive exploratory data analysis (EDA) to understand feature distributions, correlations, and relationships with the target variable.
- Implemented and compared multiple models including Linear Regression, Decision Tree, Random Forest, Gradient Boosting, and several neural network architectures (Simple, Deep, Wide and Deep).
- Presented detailed visualizations of model performance and feature importance to aid in model interpretation and selection.

Supercell and Alloy Structure Development using VESTA *(May 2024)*
Summer Project ,Prof. Appala Naidu Gandi

- Constructed supercell models with 20 Å vacuum slabs for **Al (FCC)**, **Cr (BCC)**, and **Ti (HCP)** surfaces to study structural stability and surface properties.
- Developed and analyzed **Cu-based alloys** (**Brass** and **Bronze**) by integrating Zn and Sn atoms into Cu slabs to evaluate compositional effects on crystal structure.

Object Detection and Reporting System using YOLO and Text-to-Speech (TTS) *(Jan'24 - April'24)*
Prof. Arpit Khandelwal, **Github**

- Developed a real-time Object Detection and Reporting System using Python, incorporating YOLO model for object detection and gTTS for text-to-speech conversion.
- Integrated OpenCV for image processing and capturing frames from the webcam, ensuring efficient data handling.

- Deployed the system on Raspberry Pi for low-cost, energy-efficient operation, demonstrating proficiency in embedded system deployment, Python programming, and image processing.

Prediction of Grasp and Lift EEG Motion Detection *(Aug'23 - Dec'23)*
Prof. Avinash Sharma

- Executed an EEG motion detection project, utilizing neural networks to predict hand movements, such as grasping and lifting, from extensive timeseries data.
- Implemented advanced signal processing techniques, including denoising for waveform data, contributing to a deeper understanding of neural networks, signal processing, and data analysis for precise motion classification.

SKILLS

- **Programming Languages:** C/C++, Python , MATLAB , SQL
- **Computational materials:** Quantum Espresso, VESTA, GNU Plot, XCrysden , MD++ , LAMMPS , OVITO
- **Characterization:** SEM , XRD , FT-IR Spectroscopy , UV-Vis Spectroscopy , Optical Microscopy
- **Crystal Plasticity:** DAMASK , Dream3Dnx , Paraview , NEPER , OIM
- **Materials Informatics:** Materials project , Pymatgen , Matminer , gplearn , SHAP
- **Testing and Processing:** Hardness Testing , Tensile Testing , Precision Cutting , Grinding , Polishing , Failure Analysis , EIS , Spin Coating
- **Web Development:** HTML, CSS, Bootstrap
- **Software and Libraries:** Pandas, Numpy, Matplotlib, SeaBorn, Scikit-Learn, PyTorch, TensorFlow, Keras, Open-CV, Streamlit, Origin , FIGMA
- **Soft Skills:** Leadership, Analytical and Strategic thinking, Problem-Solving, Reasoning, Emotional Intelligence, Communication

POSITIONS OF RESPONSIBILITY

- **Student Guide, Student Well-being Committee (AY 2023–24)** — Mentored 12 freshmen to help them adapt academically and socially; selected among 50 guides from 500 applicants.
- **Assistant Head, Informals – Prometeo'23** — Led coordination and execution of a 3-day institute event; managed budget and vendor communication.
- **Volunteer, Public Relations – Prometeo'22** — Engaged with sponsors and attendees, enhancing event visibility and communication.

RELEVANT COURSES

Introduction to Machine Learning, Data Structures and Algorithms, Scientific Computations, Introductory Condensed Matter Physics, Materials for Energy Conversion and Storage, Materials at Equilibrium, Polymers, Physical Metallurgy, Materials Characterization, Electronic Materials, Introduction to Dislocation Dynamics, Mechanical Behaviour of Materials, Phase Transformations, Communication Skills, Iron and Steel Making, Extraction of Non-Ferrous Metals, Smart Materials, Crystal Plasticity and Its Applications, Computational Modelling of Materials, Processing Microstructure and Properties of Steels, Materials Processing and Manufacturing