

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, Akhil Garg. *Uncertainty-Aware Prediction of Mechanical Properties in 2D Materials Using Random Forest and Monte Carlo Simulations.* Submitted to *Computational Materials Science*, 2025.

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

- In-situ Monitoring and Dimensional Analysis of Additive Manufacturing (Deep Learning, 3D Reconstruction):** Developed an in-situ monitoring system for 3D-printed components using deep learning to perform real-time 3D reconstruction and dimensional analysis of additively manufactured parts.
- Layer Determination in 2D TMD Materials (Deep Learning, Materials Science):** Utilized deep learning to accurately determine the number of layers in two-dimensional transition metal dichalcogenides (TMD) materials. (Ongoing)
- 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.

PROJECTS

- **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 Gandhi
 - 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 Gandhi
 - 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).
 - Achieved the best performance with the Random Forest model, with an RMSE of 0.1207, MAE of 0.0586, and R² of 92.10%.
 - Utilized TensorFlow for building neural networks, Scikit-learn for implementing other machine learning models, and various data processing techniques.
 - Presented detailed visualizations of model performance and feature importance to aid in model interpretation and selection.
- **Supercell Structure Creation for Surface Property Studies** (May'24)
Summer Project, Mentor: Prof. Appala Naidu Gandhi
 - Developed advanced supercell structures using VESTA.
 - Aluminum (FCC): Constructed a supercell with 20 Å vacuum for a slab containing 12 (111) planes.
 - Chromium (BCC): Designed a supercell with 20 Å vacuum for a slab containing 12 (110) planes.
 - Titanium (HCP): Engineered a supercell with 20 Å vacuum for a slab containing 12 (0001) planes.
- **Alloy Crystal Development and Analysis** (May'24)
Prof. Appala Naidu Gandhi
 - Developed advanced alloy structures using VESTA.
 - Brass (FCC): Created a supercell by integrating 69% Copper and 29% Zinc into a slab of Cu.
 - Bronze (FCC): Developed a supercell by adding 88% Copper and 12% Tin to a slab of Cu.
 - Successfully analyzed the resulting alloy crystals to determine structural properties.
- **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.

• **Book Recommendation System**

(Dec'23 - Jan'24)

Self Project, [GitHub](#), [Live Link](#)

- Developed a book recommendation system using Flask, machine learning, and data processing techniques.
- Designed an intuitive interface with HTML, CSS, and Bootstrap.
- Implemented personalized recommendations based on user preferences and historical data using machine learning algorithms. Utilized Flask for backend development and pickle for model serialization. Successfully deployed the application, showcasing proficiency in web development and machine learning.

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

POSITION OF RESPONSIBILITY AND VOLUNTEERING

- **Student Guide, Student Well-being Committee** (AY 2023-2024)
 - * Guided and mentored **12 freshmen** students in acclimatizing to the environment of the Institute.
 - * Selected as one of 50 students from a pool of 500 candidates
 - * Assisted them with their academics by arranging meetings with their mentors while maintaining a positive rapport.
- **Assistant Head Informals, Prometeo'23** (AY 2023-2024)
 - * Spearheaded the coordination and execution of a dynamic 3-day event, overseeing tasks ranging from budget management to vendor communication. Responsibilities encompass strategic budget utilization, ensuring seamless coordination with vendors, and overall event execution.
- **Volunteer Public Relations, Prometeo'22** (AY 2023-2024)
 - * As a member of the Public Relations team, actively engaged in fostering positive relationships with attendees, sponsors, and the media, enhancing the overall event experience. This experience significantly honed my communication skills through strategic interactions and effective promotional efforts.

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