Rushik Desai

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Summary

PhD candidate with a strong background in **solid state physics** and **atomistic simulations**. Skilled in Python, atomistic and nanoscale modeling with experience in **automated workflow management** for HPC systems, with experience in setting up **Kubernetes and SQL-databases**. Experienced in AI/ML methods, specifically focusing on **property prediction and force-field development**. Developed open-source tools to make simulations pervasive on nanoHUB (check out my tools). Seeking internships in applied ML for novel energy devices.

Education

Purdue University, West Lafayette, IN, USA   *2026*
Ph.D. in Materials Engineering (MSE) | Advisor: Prof. Alejandro Strachan and Prof. Arun Mannodi | GPA: 3.23/4.00
Relevant courses: Atomistic View of Materials: Theory, Modeling And Simulations | Introduction To Materials Modeling And Informatics | Optimization | Solid-State Devices | Scientific Machine Learning

Indian Institute of Technology Gandhinagar (IIT GN), India   *2023*
B.Tech. in Materials Engineering | GPA: 9.02/10.00
Relevant courses: Solid Mechanics | Mechanical Behavior of Materials | Processing and Characterization

Technical Skills

- **Computational Tools:** Machine Learning (ML), Density Functional Theory (DFT), and Molecular Dynamics
- **Programming Languages:** Python, Linux, Shell scripting, MATLAB
- **Software and Packages:** PyTorch, Scikit-learn, Pandas, High-Performance Computing, VASP, Quantum Espresso, LAMMPS
- **Experimental Tools:** XRD, Optical Spectroscopy, SEM, Materials Processing, Thin Films Processing

Professional Experience

Graduate Research Assistant | Purdue University | Advisor: Prof. Alejandro Strachan and Prof. Arun Mannodi
Broad Topics: Defect Modeling | Perovskites | GNNs | ML and optimization

⇒ **Material-Device Co-design for High-temperature Piezoelectric Sensors**   *July'25-Ongoing*
  · Data-driven curation of Langasite-based material properties.
  · Developing an **active learning pipeline** by training predictive GNNs to obtain tensorial properties.
  · Utilizing material properties to **optimize device performance** using COMSOL.

⇒ **FAIR Perovskite Database**   *Aug'23-Ongoing*
  · Curating data to create **the largest perovskite and perovskite-inspired material dataset**.
  · Storing everything in a **FAIR (Findable, Accessible, Interoperable, and Reusable)** database for community use.
  · Created **automated workflows** to extract important perovskite properties integrable into **ML-pipelines**.
  · Trained predictive models on this database to predict **synthesizability** of different perovskites.

⇒ **Exploring the Defect Landscape of BaZrS$_3$**   *May'24-Ongoing*
  · Performed **high-fidelity point defect calculations** for promising photovoltaic BaZrS$_3$.
  · Obtained carrier properties matching with experiments and highlighted the reason for poor device efficiency.
  · High-throughput dopant calculations revealed novel **dopants to make material p-type**, the first study of its kind.

Research Intern | University of Manitoba | Advisor: Prof. Georg Schreckenbach   *May'22-Jul'22*
  ⇒ **Band-gap modulation of novel 2D Materials**
  · Using DFT, band-gap, phonon, and DOS calculations were performed for stand-alone **2D materials and 2D heterostructures** using VASP, Phonopy, and QE.

- · Employed methods like applying strain, electric field, and doping to modulate the band gap of **silicene-germanene heterostructures and heterojunctions**
- · Worked on a Titanium Carbo-Chalcogenide and did calculations using epw with QE to understand its **superconducting properties**.

Undergraduate Research Assistant | IIT GN | Advisor: Prof. Raghavan Ranganathan *Aug'21-May'22*
⇒ **Viscoelastic Study of Polyethylene Nanocomposites**
- · Constructed a **coarse-grained model for the polyethylene-graphene system**. Used hybrid force fields to parameterize the nonbonded interactions between polyethylene and graphene using MD in the LAMMPS package.
- · Simulated **nanocomposites with multiple graphene sheets** to understand the difference in properties due to nanoconfinement effects.

Experimental Work | Broad Topics: Thin Film Fabrication | Materials Characterization
Undergraduate Research Assistant | IIT GN | Advisor: Prof. Emila Panda *Aug'22-Dec'22*
⇒ **Developing a buffer layer for VO_2 thin film coatings**
- · Worked on developing a **mid-far infrared transparent buffer layer** of rutile TiO_2 for VO_2-based coatings
- · **Deposited TiO2 films using the RF Magnetron Sputtering Device** and performed temperature-dependent phase studies.
- · Performed **XRD** to get the phase of the film and **UV-Vis-NIR** to understand the optical properties.

Publications ——————————————————— († **first or co-first author**)

⇒ Biswas, M.; **Desai, R.**[†]; Bidna, G.; Mannodi-Kanakkithodi, A. Unified Graph-Based Interatomic Potential for Perovskite Structure Optimization. ChemRxiv July 14, 2025. https://doi.org/10.26434/chemrxiv-2025-g9sb9. (Under review in JCIM)

⇒ Marshall, J.; Sanchez, S.; **Desai, R.**; Foadian, E.; Pratiush, U.; Mannodi-Kanakkithodi, A.; Kalinin, S. V.; Ahmadi, M. POLARIS: Perovskite Optimization Using LLM-Assisted Refinement and Intelligent Screening. ChemRxiv June 10, 2025. https://doi.org/10.26434/chemrxiv-2025-qqchd-v2. (Under Review in Digital Discovery)

⇒ **Desai, R.**[†]; Agarwal, S.; Vincent, K. C.; Strachan, A.; Agrawal, R.; Mannodi-Kanakkithodi, A. Exploring the Defect Landscape and Dopability of Chalcogenide Perovskite BaZrS3. J. Phys. Chem. C 2025, 129 (16), 7967–7976. https://doi.org/10.1021/acs.jpcc.5c01597.

⇒ Biswas, M.; **Desai, R.**[†]; Mannodi-Kanakkithodi, A. Screening of Novel Halide Perovskites for Photocatalytic Water Splitting Using Multi-Fidelity Machine Learning. Physical Chemistry Chemical Physics 2024, 26 (35), 23177–23188. https://doi.org/10.1039/D4CP02330G.

Conferences ——————————————————————

Materials Research Society Fall Meeting *Dec'24*
⇒ Presented a talk on FAIR database curation for halide perovskites, showcasing our database and workflows along with the tool demo.

Materials Research Society Fall Meeting *Dec'25*
⇒ Accepted for a talk on FAIR workflows for understanding properties and synthesizability of perovskite compositions.

Leadership & Mentorship Experience ——————————

Structure and Properties of Materials, Teaching Assistant, Purdue University *Fall'24*
⇒ Conducted tutorials for 80 students on different topics, ranging from XRD to phase diagrams.

Graduate Research Mentor, Purdue University *Fall'24, Spring'25, Summer'25*
⇒ Mentored a junior undergrads in curating datasets, training models, and developing tools on nanoHUB
⇒ Cultivated scientific curiosity conveyed advanced research concepts to achieve accurate predictive models

Awards and Achievements ——————————————

⇒ Awarded **Best Poster Presentation** at Materials Research Data Alliance (MaRDA) Annual Meeting *2024*
⇒ Computing time allocation, **Argonne National Laboratory Cluster (2024, 2025), NSF ACCESS Anvil Cluster (2025)**.
⇒ Awarded **Mitacs Globalink Fellowship** to conduct 12 weeks of research in Canada *2022*