

Shiba Sankar Dash

M.Tech (Research), Computational Materials Science

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EDUCATION

M.Tech (Research), Materials Engineering

Indian Institute of Science (IISc), Bangalore

Aug 2023 – April 2026 (expected)

CGPA: 8.2/10.0; Completed 11 advanced graduate courses

B.Tech, Ceramic Engineering (Minor in Metallurgy)

National Institute of Technology (NIT) Rourkela

Aug 2018 – May 2022

CGPA: 8.18/10.0; Minor GPA: 8.29/10.0 (*only student in cohort to complete dual curriculum*)

RESEARCH INTERESTS

Atomistic and multiscale modelling of defect–solute interactions, elastic anisotropy effects, and segregation-driven changes in mobility and failure, integrated with SEM/EDS-based microstructure characterization; extending DFT+ML frameworks to multicomponent alloys, stacking-fault physics, and high-temperature structural materials

RESEARCH EXPERIENCE

M.Tech Thesis: Hydrogen–Dislocation Interactions in Nickel using DFT and Machine Learning

Jun 2024 – Present

Indian Institute of Science (IISc), Bangalore | Advisor: Prof. S. Karthikeyan

- Performed **200+ DFT calculations** (VASP) to map hydrogen segregation across dislocation strain fields in Ni, establishing a robust dataset for ML training.
- Built Random Forest regression model ($R^2 \sim 0.99$) revealing that **hydrostatic stress dominates H-segregation** (not shear), clarifying a key atomistic embrittlement mechanism.
- Demonstrated that incorporating **elastic anisotropy increases predicted peak H concentrations by 40–50 %** at edge dislocations, highlighting a frequently overlooked factor in failure models.
- Identified **Suzuki-type segregation** to stacking faults leading to unexpectedly high H-trapping at screw dislocations, with direct implications for cross-slip and failure mode selection.
- Results presented as an **oral talk at H2MSE 2025** (Germany); **manuscript in preparation**.

Phase-Field Modelling Project: Spinodal Decomposition in Binary Alloys

Jan 2024 – Apr 2024

Indian Institute of Science (IISc), Bangalore

- Implemented a Cahn–Hilliard phase-field model using **MicroSim** to study spinodal decomposition and coarsening, tuning free-energy parameters and gradient-energy coefficients.
- Gained mesoscale intuition linking diffusion kinetics and interfacial energy to microstructural evolution—directly complementing atomistic segregation trends from my DFT work.

Undergraduate Project: Toughening Mechanisms in Soda-Lime Glass

Aug 2021 – Apr 2022

NIT Rourkela

- Investigated thermal and chemical toughening routes; **achieved 25 % increase in fracture toughness** through optimized ion-exchange processing.
- Designed and built a custom multi-zone furnace with laboratory technicians to enable controlled processing experiments, demonstrating hands-on problem-solving.

SKILLS AND TECHNICAL PROFICIENCIES

Computational & Atomistic: VASP (advanced DFT for defect energetics), LAMMPS (MD for dislocation/crack-tip evolution), Quantum Espresso

Mesoscale & Continuum: MicroSim (phase-field), ANSYS (FEM); strong foundation in dislocation dynamics and microstructure evolution

Programming & Data Science: Python (NumPy, Pandas, scikit-learn), MATLAB, bash/Linux, data visualization (Origin, VESTA, OVITO)

Experimental & Characterization: SEM (fractography), XRD, Split Hopkinson Pressure Bar (SHPB) testing

PUBLICATIONS AND PRESENTATIONS

- **Oral Presentation:** “A DFT study of hydrogen interstitial solute interaction with dislocations in nickel,” **1st International Conference on Hydrogen in Materials Science and Engineering (H2MSE 2025)**, Bonn, Germany.
- IISc Materials Engineering Student Symposium, March 2025.

INDUSTRY EXPERIENCE

Graduate Engineer Trainee – Steelmaking Operations *Jun 2022 – Feb 2023*
ArcelorMittal Nippon Steel India (AM/NS), Hazira Plant

- Analyzed **50+ refractory wear audits**, correlating thermal cycles and slag chemistry with specific degradation mechanisms; recommended process adjustments that extended lining life by ~15 %.
- Investigated root causes of hydrogen-induced cracking in interstitial-free steels by monitoring **200+ slab casts**; traced H-ingress to specific processing stages.
- Collaborated with multilingual furnace operators to implement real-time adjustments, reducing casting defects by 10% and demonstrating effective cross-disciplinary communication.

Summer Intern – Rourkela Steel Plant (SAIL) *Jun 2021 – Jul 2021*

- Observed integrated steelmaking workflows from blast furnace to rolling mill; documented quality control protocols for defect analysis.

AWARDS AND HONORS

- **Best Presentation Award** – IISc Open Day 2025 (top 5% of presenters)
- **GATE Metallurgy** – All India Rank 218 (Top ~2 %)
- **Runner-up** – IIM Rourkela Steel Plant Chapter Materials Design Competition 2022

PERSONAL INTERESTS

Chess, cricket, cycling, endurance sports, and science communication.

LANGUAGES

English (fluent), Hindi (fluent), Odia (native)

REFERENCES

Prof. S. Karthikeyan

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Prof. Praveen Kumar

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