

Sachin Poudel, Ph.D. Candidate

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Research Interests

- Multi-Principal Element Alloys
- Machine Learning
- Advanced Functional Materials
- Microstructural Evolution
- Scale-Bridging Simulations
- Phase Field Modeling
- Computational Materials Science

Education

- Feb 2023 – Present 🔦 **Ph.D. in Mechanical Engineering**, Silesian University of Technology, Poland.
Thesis: *Scale-Bridging Computational and Data-Driven Design of Microstructures in Multicomponent Alloys for Advanced Functional Materials*
- Aug 2020 – Sep 2022 🔦 **M.Sc. in Mechanical Design and Manufacturing**, Tribhuvan University, IOE, Thapathali Campus, Nepal.
Thesis: *Towards Accelerated Design of Multi-Principal Element Alloys with Optimized Hardness and Elongation Features by an Ensemble of Neural Network*
- Nov 2014 – Oct 2018 🔦 **B.E. in Mechanical Engineering**, Tribhuvan University, IOE, Thapathali Campus, Nepal.
Project: *Design, Fabrication, and Testing of Banana Fibre Extraction Machine*

Skills

- Computational Methods 🔦 Phase-Field Modeling, Density Functional Theory, Finite Element Methods, Multi-Scale Simulations, Non-linear Electrochemical Modeling
- Machine Learning 🔦 Data Preprocessing & Featurization (Matminer, Pymatgen, Magpie featurization, PCA, Pearson Correlation), Neural Networks (TensorFlow/PyTorch), Ensemble Methods, Hyperparameter Tuning, MeshGraphNet
- Programming Languages 🔦 Python (NumPy, SciPy, scikit-learn, Streamlit), MATLAB, C++, Fortran, Data Visualization & Analysis (Matplotlib, Plotly, Pandas)
- Software & Frameworks 🔦 MOOSE, Elmer, Quantum Espresso, ANSYS, Git, Linux
- Languages 🔦 Strong reading, writing, and speaking competencies for English, Nepali

Research Experience

Phase-Field Modeling & Multi-Scale Coupling

- ◆ Formulated and implemented multi-component phase-field models in MOOSE, integrating bulk, interfacial, and elastic energy contributions.
- ◆ Embedded DFT-computed temperature-dependent elastic constants and to simulate Al-Cu-Ni microstructure evolution, revealing 18.2% grain area deviation at 723K compared to 0K elastic constants.
- ◆ Developed non-linear electrochemical ion migration modules by coupling Butler-Volmer kinetics to phase-field evolution, elucidating Li-ion dendrite nucleation and growth mechanisms.

Research Experience (continued)

Piezoelectric Materials Fine-Tuning via ML, Crystallography & FEM

- ◆ Architected PiezoTensorNet: hierarchical neural classifiers for crystal point group identification and modular regression ensembles predicting piezoelectric tensors from dopant-enhanced crystallographic inputs.
- ◆ Integrated tensor predictions into FEM simulations of AlN MEMS devices to optimize dopant concentrations and Euler orientations, achieving $5.96\times$ power density gains and $>92\%$ accuracy.

Data-Driven Materials Design Pipeline

- ◆ Aggregated, normalized, and featurized heterogeneous datasets of alloy compositions, processing parameters, and performance metrics; applied PCA and Pearson correlation for feature selection.
- ◆ Trained and optimized artificial neural networks and ensemble regressors, achieving cross-validated $R^2 > 0.88$ for hardness and elongation predictions.

Synergetic Optimization of MPEA Mechanical Properties

- ◆ Clustered manufacturing routes (casting, wrought, powder metallurgy, annealing) and employed scale-invariant normalization to identify dual-dopant synergies in multi-principal element alloys.
- ◆ Predicted and experimentally validated compositions yielding $>15\%$ concurrent gains in hardness and elongation for Ti-doped ZrHfNb and $\text{Cr}_{0.5}\text{W}_{0.3}(\text{VNbTa})_{0.2}$ alloys.

Hybrid Computational–Data & Web Frameworks

- ◆ Developed closed-loop pipelines coupling phase-field outputs with machine learning surrogates, accelerating parameter calibration and enhancing predictive fidelity.
- ◆ Deployed AlloyManufacturingNet and PiezoTensorNet as Streamlit web applications with RESTful back-ends, enabling real-time property forecasting, composition optimization, and interactive visualization.

Functional Device Applications in Energy Storage & Conversion

- ◆ Applied integrated modeling frameworks to design and optimize functional devices: simulated dendrite evolution for Li-ion batteries, and enhancing piezoelectric MEMS actuator voltage generation by alloying a crystallographic rotation.





Research Publications

Journal Articles






- 1 **S. Poudel**, N. Moelans, R. Thapa, A. Timofiejczuk, D. Panthi, and A. Kunwar, “Unraveling elastochemical effects in microstructural evolution of al–cu–ni system through dft-informed multi-phase field simulations,” *International Journal of Solids and Structures*, vol. 300, p. 112 894, 2024. [DOI: 10.1016/j.ijsolstr.2024.112894](https://doi.org/10.1016/j.ijsolstr.2024.112894).
- 2 **S. Poudel**, U. Subedi, M. O. Hamid, *et al.*, “Alloymanufacturingnet for discovery and design of hardness-elongation synergy in multi-principal element alloys,” *Engineering Applications of Artificial Intelligence*, vol. 132, p. 107 902, 2024. [DOI: 10.1016/j.engappai.2024.107902](https://doi.org/10.1016/j.engappai.2024.107902).
- 3 **S. Poudel**, R. Thapa, R. Basnet, A. Timofiejczuk, and A. Kunwar, “Piezotensornet: Crystallography informed multi-scale hierarchical machine learning model for rapid piezoelectric performance finetuning,” *Applied Energy*, vol. 361, p. 122 901, 2024. [DOI: 10.1016/j.apenergy.2024.122901](https://doi.org/10.1016/j.apenergy.2024.122901).

- 4 R. Thapa, **S. Poudel**, K. Krukiewicz, and A. Kunwar, "A topical review on ai-interlinked biodomain sensors for multi-purpose applications," *Measurement*, vol. 227, p. 114 123, 2024. [DOI: 10.1016/j.measurement.2024.114123](https://doi.org/10.1016/j.measurement.2024.114123).
- 5 U. Subedi, **S. Poudel**, K. Gyanwali, Y. Amorim Coutinho, G. Matula, and A. Kunwar, "State-of-the-art review on the aspects of martensitic alloys studied via machine learning," *Metals*, vol. 12, no. 11, p. 1884, 2022. [DOI: 10.3390/met12111884](https://doi.org/10.3390/met12111884).
- 6 **S. Poudel**, S. Chapai, R. K. Subedi, T. R. Giri, and S. Adhikari, "Design, fabrication, and testing of banana fibre extraction machine," *Journal of Innovations in Engineering Education*, vol. 2, no. 1, pp. 165–173, 2019. [DOI: 10.3126/jiee.v2i1.36668](https://doi.org/10.3126/jiee.v2i1.36668).

Conference Presentations



- 19 – 23 May 2024  The 5th International Symposium on Phase-Field Modelling in Materials Science, Zhejiang University, Hangzhou, China.
"A computational model for examining the role of externally applied stress on dendrite growth pattern in solid state Lithium-ion batteries". (Oral Presentation)
- 3 – 7 Sep 2023  Euromat23, Frankfurt, Germany "Phase field evolution in Ni-YSZ Fuel Cells with Temperature-Dependent Elasticity". (Oral Presentation)
- 19 – 22 Oct 2022  12th IOE Graduate Conference, Thapathali Campus, Nepal "Towards Accelerated Design of Multi-Principal Element Alloys with Optimized Hardness and Elongation Features by an Ensemble of Neural Network [ID: 12308]". (Oral Presentation)
- 05-06 April 2019  Fifth Graduate Conference- Himalayan Knowledge Conclave 2019, Kathmandu University, Nepal. "Design, Fabrication and Testing of Banana Fibre Extraction Machine". (Poster Presentation)

Employment History

- April 2023 – Present  **Graduate Researcher**, Silesian University of Technology.
Research team member in the National Science Centre (NCN), Poland, funded project.
- Feb 2022 – Jan 2023  **Lecturer**, COSMOS College of Management and Technology, Nepal.
Delivered lectures and instructed in laboratory on mechanical engineering subjects: Thermal Science (MEC 111) and Engineering Drawing (MEC 120).
- Nov 2021 – Feb 2023  **Teaching Assistant**, IOE, Thapathali Campus, Tribhuvan University, Nepal.
Teaching core mechanical engineering courses: Engineering Drawing I (ME401), Engineering Drawing II (ME451), Computer Aided Drawing (ME 505).
- Jun 2019 – Nov 2021  **Mechanical Design Engineer**, Calcgen Solutions, Nepal.
Conducted finite element analysis and stress analysis of pressure vessel components. Performed mechanical calculations and drafting of pressure vessels based on ASME Section VIII.
- Sep 2018 – Dec 2018  **Intern**, Nepal Airlines Corporation, Nepal.
Diagnosed aircraft vehicles. Assisted in the repair and maintenance of various aircraft models.

Professional Achievements and Engagements

Awards and Recognitions

- 2024  **Rector's Grant, Silesian University of Technology, Poland.** Pro-quality competition for rector's grants for highly scored publications, granted patents, acquired projects, or scientific and research work
- 2023  **University Grants Commission, Nepal.** University Grants Commission (UGC) Master Research Support Award (Award No: MRS-78-79-Engg-10)

Workshops and Events

- 2 Jan – 5 Jan 2019  **Swiss-Nepal Technology Transfer Workshop 2019.** Organized by the Nepalese Scientific Association in Switzerland (NepSas)
- 4 Feb – 6 Feb 2016  **MechTRIX 7.0.** 7th National Mechanical Engineering Exhibition 2073