

Dr. Shakti Prasad Padhy, PhD

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🏠 Shakti Prasad Padhy

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RESEARCH INTEREST

My research focuses on leveraging AI-driven frameworks to revolutionize materials discovery and design. By integrating advanced machine learning algorithms, such as generative AI and multi-objective optimization, with high-throughput experimental techniques, I aim to accelerate the development of novel materials tailored for renewable energy, aerospace, and biomedical applications. I am particularly passionate about addressing challenges in processing-structure-property-performance relationships, sustainability, and scalability, enabling eco-friendly synthesis and industrial adoption of high-performance materials. My future work aspires to establish self-driving laboratory workflows for autonomous synthesis and real-time decision-making to explore underutilized material systems and advance energy-efficient technologies.

SKILLS SUMMARY

- **Experimental:** Additive manufacturing or 3D Printing of metals, Chemical synthesis of nanoparticles, DC Magnetron co-sputtering, Atomic Force Microscopy (AFM), High Energy Ball milling, High Throughput Spark Plasma Sintering (HT-SPS), High Throughput X-ray Diffractometer (HT-XRD), Arc Melting, Scanning Electron Microscope (SEM), Electron Backscatter Diffraction (EBSD), Vibrating Sample Magnetometer (VSM), Physical Property Measurement System (PPMS), High Throughput four-point probe (HT-FPP), Nanoindentation
- **Languages & Tools:** Python, MATLAB, C, SQL, Git, HTML, CSS
- **Packages:** TensorFlow, PyTorch, Keras, Tensorflow-GAN, KerasTuner, NumPy, Pandas, Scikit-learn, XGBoost, SHAP, LIME, OpenCV, NLTK, Scipy, Seaborn, Matplotlib, Plotly, GPax, Scikit-image, Scikit-Optimize, Optuna, PySwarms

WORK EXPERIENCE

- **Incoming Postdoctoral Researcher** May 2025 - Present
Texas A&M University *College Station, Texas, USA*
- **Research Fellow** May 2024 - Apr 2025
Nanyang Technological University *Singapore, Singapore*
 - Lead a collaboration with Panasonic to develop soft magnetic materials using additive manufacturing for electric motors, delivering results under strict deadlines and providing timely updates through reports and presentations.
 - Mentored a graduate and a Masters student in developing Multi-objective Multi-step Look-ahead Bayesian Optimization (MoMsLaBO) for automated batch experiments, significantly enhancing materials design efficiency.
 - Guided two PhD students in scaling up Mn-Zn ferrite synthesis by optimizing process parameters through machine learning to achieve high-impact research outcomes.
 - **Techniques used:** Additive Manufacturing, SEM, EBSD, HT-XRD, HT-FPP, Vickers Hardness, VSM, PPMS, Python, ML/DL techniques
- **Post-doctoral Research Associate** Sep 2023 - Feb 2024
University of Tennessee Knoxville *Knoxville, Tennessee, USA*
 - Co-developed a cost- and physics-aware Bayesian optimization approach for nanoindentation experiments on high entropy refractory alloys, reducing experimental time and improving overall research efficiency.
 - Conducted structural analysis of combinatorial thin film Raman spectroscopy data using PCA, NMF, and BLU, resulting in more accurate data interpretation and actionable insights on material properties.
 - Led nanoindentation and AFM experiments on high entropy refractory alloys in collaboration with postdoctoral fellows, enhancing material property analysis and research outcomes through effective teamwork.
 - **Techniques used:** Nanoindentation, Magnetron co-sputtering, AFM, Python, ML techniques
- **Research Assistant** Jan 2023 - Aug 2023
Nanyang Technological University *Singapore, Singapore*
 - Applied transfer learning on a pre-developed multi-output predictive model for adapting to particular experimental method using limited data and improved model's performance by 57.7%.
 - Conducted synthesis experiments on ML-designed Fe-Co-Ni alloys, identifying a synthesis method with only 14% deviation from ML predictions, achieving accurate and reliable results through collaboration with a PhD student and research fellows.
- **Project Intern** Aug 2018 - Dec 2018
Birla Institute of Technology & Science Pilani, Hyderabad Campus *Hyderabad, India*
 - Developed a protocol to conjugate Cathepsin D antibody to stable 49 nm gold nanoparticles for cancer detection via saliva.
 - Experimented Turkevich, chitosan reduction, and polyvinylpyrrolidone reduction synthesis methods for gold nanoparticles.
 - **Techniques used:** Chemical synthesis of nanoparticles, Zeta potential analyzer
- **Bachelor Thesis Intern** Jan 2018 - May 2018
Institute of Nanotechnology, Karlsruhe Institute of Technology *Karlsruhe, Germany*
 - Developed a protocol for patterning an organometallic photo-responsive polymer gel by optimizing its viscosity.
 - Studied the effect of printing parameters on the pattern size.
 - **Techniques used:** Dip-pen nanolithography, microchannel cantilever spotting, AFM.

EDUCATION

- **Doctor of Philosophy, Materials Science and Engineering** Jan 2019 - Dec 2023
Nanyang Technological University
Supervisor: Prof. Raju V. Ramanujan
Thesis: Accelerated Development of Soft Magnetic Materials
- **Bachelor in Engineering (Honors) Chemical Engineering** Aug 2014 - July 2018
Birla Institute of Technology and Science (CGPA: 8.3/10)
Minor in Materials Science and Engineering
Supervisor: PD Dr. Dr. Michael Hirtz, Karlsruhe Institute of Technology
Thesis: Surface Functionalization via microchannel cantilever spotting and dip-pen nanolithography

SELECTED RESEARCH PROJECTS

- **Probabilistic AI for the finite element driven homogenization of the three-phase particulate composites with pores (Feb 2025 - Present)**
 - Developed a probabilistic ML workflow using various quantile regressors and Bayesian based regressors to predict elastic properties of homogenized three-phase particulate composites with pores, using finite element analysis (FEA).
 - Collaborated with two researchers to source and preprocess FEA data, identifying the optimal ML approach and fostering teamwork throughout the project.
 - Applied SHAP and LIME to provide interpretable insights along with model's prediction uncertainty for informed design strategy of composites for practical applications.
 - **Skills:** Python, Scikit-Learn, sklearn_quantile, TensorFlow, Keras, SHAP, LIME, Pandas, Numpy, Seaborn, Matplotlib
- **Explainable AI for Predicting Natural Frequencies of Bidirectional Functionally Graded Cracked Plates (Nov 2023 - Oct 2024)**
 - Developed an explainable ML workflow with computation time analysis to predict natural frequencies of bidirectional functionally graded plates with cracks, using finite element analysis (FEA).
 - Collaborated with two researchers to source and preprocess FEA data, identifying the optimal ML approach and fostering teamwork throughout the project.
 - Applied SHAP to simplify complex model predictions, providing clear and interpretable insights for practical applications.
 - Managed project timelines effectively, delivering the predictive model and comprehensive results within deadlines.
 - **Skills:** Python, Scikit-Learn, XGBoost, TensorFlow, Keras, SHAP, Pandas, Numpy, Seaborn, Matplotlib
- **Integrated Design Framework for Titanium Aluminides Through Explainable ML and MOBO (Jan 2022 - Jun 2024)**
 - Collaborated with a team of researchers, providing guidance and expertise to convert unstructured data from literature into a structured format, preparing it for further analysis.
 - Implemented the developed ML-based imputation strategy to fill gaps in the dataset, ensuring data completeness and accuracy while adapting to evolving project needs.
 - Developed and trained multi-input, multi-output models, generating accurate predictions of complex material properties.
 - Implemented multi-objective Bayesian optimization along with explainable ML techniques, optimizing alloy composition and testing conditions to meet project goals.
 - **Skills:** Python, Scikit-Learn, Scikit-Optimize, TensorFlow, Keras, KerasTuner, SHAP, Pandas, Numpy, Seaborn, Matplotlib
- **Inverse design of multi-property Fe-Co-Ni alloys using ML and multi-objective Bayesian optimization (MOBO)(Jan 2019 - May 2024)**
 - Converted unstructured data from literature into structured format, preparing a cleaned dataset for further analysis and imputation.
 - Developed an imputation strategy to address gaps in the structured dataset, ensuring data accuracy and completeness for effective modeling.
 - Trained and implemented multi-input, multi-output models using tree-based and neural network approaches to predict multiple key material properties.
 - Applied multi-objective Bayesian optimization to the inverse design of alloy compositions, refining alloy properties for optimized performance.
 - Explored PySwarm optimization algorithms, experimenting with additional approaches to improve the alloy design process.
 - **Skills:** Python, Scikit-Learn, Scikit-Optimize, TensorFlow, Keras, KerasTuner, Pandas, Numpy, Scipy, Seaborn, Matplotlib, Pyplot, Optuna, PySwarms
- **Accelerated development of Fe-Co-Ni alloys using Hyperheuristic Combinatorial Flow Synthesis device (Jan 2021 - Nov 2023)**
 - Assisted in designing a multi-channel flow synthesis device and optimized flow rate regimes to achieve gradients in output solutions.
 - Designed experiments for the combinatorial synthesis of Fe-Co-Ni alloy powders, systematically exploring the ternary compositional space.
 - Developed a high-throughput method to sinter powder alloys, creating compositionally graded cylindrical bulk samples for streamlined testing.

- Conducted high-throughput analysis of electrical, magnetic, and mechanical properties of bulk samples, identifying 3 compositions with an optimal property combination for advanced applications.
 - Skills:** Device design, Device optimization, Ideation & design of experiments, Chemical synthesis of alloy nanoparticles, High Throughput Spark Plasma Sintering, High Throughput X-ray Diffractometer, Scanning Electron Microscopy, High Throughput four-point probe, Vibrating Sample Magnetometer, Nanoindentation, Vickers hardness
- Rapid multi-property assessment of compositionally modulated Fe-Co-Ni thin film material libraries (Jan 2020 - Jun 2021)**
 - Synthesized compositionally modulated Fe-Co-Ni thin film material libraries under varied processing conditions using magnetron co-sputtering.
 - Accelerated the analysis of structural, electrical, magnetic, and mechanical properties across material libraries, identifying the library with the most favorable property combination.
 - Discovered a potential alloy composition with an optimal blend of properties suited for rotating electrical machine applications, contributing to advancements in material performance.
 - Skills:** Magnetron co-sputtering, High Throughput X-ray Diffractometer, Scanning Electron Microscopy, High Throughput four-point probe, Vibrating Sample Magnetometer, Nanoindentation

TEACHING EXPERIENCE

- TRA440 - High throughput methods for accelerating materials discovery, Chalmers University of Technology, Sweden (15 Nov 2024)**
 - Guest Lecture on topic "Artificial Intelligence (AI)/ Machine Learning (ML) for Accelerated Materials Discovery (AMD)" for the newly course introduced for the first time for graduate students.
 - Tutored the students on the basics of data types and machine learning types and algorithms, and the ML-based design strategies implemented for materials design and discovery.
- MS0003 - Introduction to Data Science and Artificial Intelligence, Nanyang Technological University, Singapore (Jan 2022 - May 2022 & Jan 2021 - May 2021)**
 - Tutored undergraduate students on data handling, exploratory data analysis, regression and classification algorithms, clustering algorithms, and anomaly detection and conducted hands-on training sessions.
 - Guided student teams in analyzing the data and providing innovative insights using machine learning and data visualization.
 - Designed data-related mini projects with a team of 4 Ph.D. students and course instructor.
- MS1008 - Introduction to Computational Thinking, Nanyang Technological University, Singapore (Aug 2021 - Dec 2021)**
 - Tutored undergraduate students on the programming languages, the internal operation of a computer, the programming structure of Python, and various problem-solving techniques via algorithms in Python.
 - Conducted hands-on training sessions of programming in Python.

AWARDS AND ACHIEVEMENTS

- Best Presentation Award (Silver), *IEEE Magnetics Symposium 2022*, Singapore (Sep, 2022)
Title: Machine learning and multi-objective Bayesian optimization-based design of Fe-Co-Ni magnetic alloys
- Runner's Up, *NTU MSE 3 Minute Thesis Symposium*, Singapore (May, 2022)
Title: Accelerated Magnetic Materials Development
- Featured in *MRS TV in 2022 MRS Spring Meeting*, Honolulu (May, 2022), for *Accelerated development of Fe-Co-Ni alloys using Hyperheuristic Combinatorial Flow Synthesis device*

PUBLICATIONS

Available online:

- Tan, L. P., Davidson, K. P., Cagirci, M., Xu, X., **Padhy, S. P.**, Chaudhary, V., Ramanujan, R. V. (2025). Multi-property Evaluation of Low Cu content Fe-Cu Magnetic Alloys. *Materials Research Bulletin*, 187, 113374. [📄](#)
- Mishra, P.; Zhang, M.; Kar, M.; Hellgren, M. ; Casula, M.; Lenz, B.; Chen, A.; Recatalà-Gómez, J.; **Padhy, S. P.**;.....; Duchamp, M.; Lam, Y. M.; Hippalgaonkar, K. (2025). *Synthesis of Machine Learning-Predicted Cs2PbSnI6 Double Perovskite Nanocrystals*. *ACS Nano*, 19(6), 6107–6119. [📄](#)
- Padhy, S. P.**, Mishra, S. R., Tan, L. P., Davidson, K. P., Xu, X., Chaudhary, V., Ramanujan, R. V. (2025). Robustness of Machine Learning Predictions for Fe-Co-Ni Alloys Prepared by Various Synthesis Methods. *iScience*, 28(1), 111580. [📄](#)
- Krishnan, P. S. S. R., Vas, J. V., Mishra, S. R., Xu, X., Davidson, K. P., **Padhy, S. P.**, Duchamp. M. & Ramanujan, R. V. (2025). In-situ Operando Investigations of the Thermal Instability Mechanisms of a deformed Ti-48Al alloy. *Crystal Research & Technology*. [📄](#)

- Xu, X., Tan, L. P., Davidson, K. P., **Padhy, S. P.**, Chaudhary, V., & Ramanujan, R. V. (2024). Accelerated Discovery of Multi-property Optimized Fe-Cu Alloys. *Journal of Materials Research and Technology*, 32, 3560-3572. [📄](#)
- **Padhy, S. P.**, Chaudhary, V., Lim, Y.F., Thway, M., Hippalgaonkar, K., & Ramanujan, R. V. (2024). Experimentally Validated Inverse design of Multi-Property Fe-Co-Ni alloys. *iScience*, 27(5), 109723. [📄](#)
- Hysmith, H., Foadian, E., **Padhy, S.P.**, Kalinin, S.V., Moore, R.G., Ovchinnikova, O.S. and Ahmadi, M. (2024). The future of self-driving laboratories: From Human in the Loop Interactive AI to Gamification. *Digital Discovery*, 3, 621-636. [📄](#)
- Teh, W. H., Tan, L. P., Chen, S., Wei, F., Lee, J. J., **Padhy, S. P.**, Chaudhary, V., Tan, C. C., and Ramanujan, R. V. (2024). Breaking Conventional Limits of Silicon Content in Fe-xSi Magnetic Alloys through Additive Manufacturing. *Journal of Alloys and Compounds*, 983, 173829. [📄](#)
- **Padhy, S. P.**, & Kalinin, S. V. (2023). Domain hyper-languages bring robots together and enable the machine learning community. *Device*, 4. [📄](#)
- **Padhy, S. P.**, Tan, L. P., Varma, V. B., Chaudhary, V., Tsakadze, Z., & Ramanujan, R. V. (2023). Accelerated multi-property screening of Fe-Co-Ni alloy libraries by hyper-heuristic combinatorial flow synthesis and high-throughput spark plasma sintering. *Journal of Materials Research and Technology*, 27, 2976-2988. [📄](#)
- **Padhy, S. P.**, Tsakadze, Z., Chaudhary, V., Lim, G. J., Tan, X., Lew, W. S., & Ramanujan, R. V. (2022). Rapid multi-property assessment of compositionally modulated Fe-Co-Ni thin film material libraries. *Results in Materials*, 100283. [📄](#)
- Tan, L. P., **Padhy, S. P.**, Tsakadze, Z., Chaudhary, V., & Ramanujan, R. V. (2022). Accelerated property evaluation of Ni-Co materials libraries produced by multiple processing techniques. *Journal of Materials Research and Technology*, 20, 4186-4196. [📄](#)
- Teh, W.H., Chaudhary, V., Chen, S., Lim, S.H., Wei, F., Lee, J.Y., Wang, P., **Padhy, S.P.**, Tan, C.C. & Ramanujan, R.V. (2022). High throughput multi-property evaluation of additively manufactured Co-Fe-Ni materials libraries. *Additive Manufacturing*, 58, 102983. [📄](#)

Ongoing:

- **Padhy, S.P.**, Purohit, S., Kiran, R., Explainable Artificial Intelligence for Predicting Natural Frequencies of Bidirectional Functionally Graded Cracked Plates. *Mechanics Based Design of Structures and Machines, Under Review*.
- **Padhy, S.P.**, Chaudhary, V., Zhu, R., Tsakadze, Z., Tan, L. P., Hippalgaonkar, K., and Ramanujan, R. V. Transfer Learning and High-Throughput Experiments for Multi-Property Alloy Design. *In preparation*.
- **Padhy, S. P.**, Davidson, K. P., Varma, V. B., Tan, L. P., Jhon, M. H., Sharma, V., Tan, X., Yuefan, W., Hippalgaonkar, K., & Ramanujan, R. V. Integrated Design Framework for Titanium Aluminides Through Machine Learning. *In preparation*.
- Tan, L. P., **Padhy, S. P.**, Chaudhary, V., Hippalgaonkar, K., & Ramanujan, R. V. Multi-objective optimization for Designing Fe-Si-Al alloys with Improved Multi-functional Properties. *In preparation*.

CONFERENCE/SYMPOSIUM PRESENTATIONS

- “Machine Learning in Materials Discovery: From database curation to material design”, *MSE Graduate Students’ Club Symposium, NTU, Singapore*.
- “High Throughput evaluation of magnetic alloys for energy applications”, *TMS 2023 152nd Annual Meeting & Exhibition, San Diego, USA*.
- “Machine learning prediction and experimental validation of novel materials for rotating electrical machines”, *2022 MRS Fall Meeting Symposium DS03, Boston, USA* (First Author, Poster).
- “Rapid Multi-Property Assessment of Additively Manufactured Co-Fe-Ni Alloys”, *2022 MRS Fall Meeting Symposium SF07, Boston, USA*.
- “Machine learning and multi-objective Bayesian optimization-based design of Fe-Co-Ni magnetic alloys”, *2022 IEEE Magnetism Symposium, Singapore, Singapore* (First Author, Oral).
- “Machine Learning in Materials Discovery: From database curation to material design”, *2nd International Conference on Materials for Humanity, Singapore, Singapore* (First Author, Oral).
- “Accelerated development of new high performance materials”, *2022 International Conference On Recent Advances in Functional Materials, Delhi, India*.

- “Machine Learning guided development of Fe-Co-Ni-based soft magnetic alloy with improved mechanical and electrical properties”, *2021 IEEE Magnetics Symposium*, Singapore, Singapore (First Author, Oral).
- “Data Mining based development of Fe-Co-Ni soft magnetic materials”, *2021 IEEE International Magnetics Conference*, Lyon, France (First Author, Oral).
- “Effect of process parameters on the properties of compositionally graded FeCoNi films: A High Throughput Strategy”, *2021 IEEE International Magnetics Conference*, Lyon, France.
- “Correlation between blood glucose and salivary glucose as measured by an indigenously developed glucometer: Right-Glucose”, *International Conference on Life Science Research & its Interface with Engineering and Allied Sciences (LSRIEAS-2018)*, BITS Pilani, Pilani Campus, India (First Author, Poster).

POSITION OF RESPONSIBILITY

- **NTU Materials Science & Engineering Graduate Students’ Club (Jan 2019 - Aug 2023)**
 - President (April 2022 - August 2023)
 - Vice-President (April 2021 - March 2022)
 - Secretary (April 2020 - March 2021)
 - Publicity Director (April 2019 - March 2022)
 - **Skills:** Leadership, Delegation, Social Media & Email publicity, Teamwork, Interpersonal skills, Adaptability
- **Assistant Group Leader, Prof. Raju V. Ramanujan Group at NTU (Jan 2019 - Aug 2023)**
 - Responsible for maintaining safety protocols and neatness in laboratory by delegating the work within the group members.
 - Assisting professor in conducting weekly group meetings.
- **Council Chairperson, NTU Graduate Students’ Association (April 2022 - Aug 2023)**
 - Chairing the council of presidents of 17 graduate students’ clubs.
 - Initiating event ideas to increase collaboration between different clubs.
 - Represented the council to higher management to address issues for improving campus and research life of postgraduates.

REFERENCES

- **Dr. Raju V. Ramanujan, Professor**
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- **Dr. Varun Chaudhary, Assistant Professor**
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- **Dr. Vijaykumar B. Varma, Research & Technology Scientist (PI)**
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