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Suman Itani

Ph.D. Candidate in Physics

Professional Summary

Dedicated researcher at the intersection of condensed matter physics, materials science, and artificial intelligence. Specialized in applying large language models (LLMs) and machine learning algorithms to accelerate materials discovery and predict physical properties. Experienced in designing high-quality scientific databases and automating data extraction from literature using AI-driven workflows. Proven ability to integrate computational modeling with data-centric methods to address complex scientific challenges. Experienced educator who fosters collaborative learning environments while mentoring undergraduate students.

Research Interests

- AI-driven materials informatics for automated data extraction, database development, and property prediction
- ML-driven discovery of novel high transition temperature ferromagnetic and antiferromagnetic materials—**targeting rare-earth-free permanent magnets and low-anisotropy soft magnets**
- ML-based identification of **high-T_C superconductors**, **high-performance magnetocaloric materials candidates**, and **high-ZT thermoelectric candidates** using data-driven modeling and high-performance computing

Education

2022–2027 (expected) **Ph.D. in Physics**, *University of New Hampshire*, Durham, USA
Advisor: Prof. Jiadong Zang
Concentration: Condensed Matter Physics, Materials Science, AI

2022–2025 **M.S. in Physics (GPA: 4.0)**, *University of New Hampshire*, Durham, USA
Coursework: Solid State Physics, Condensed Matter Physics, Quantum Mechanics, Statistical Physics, High Performance Computing (Audited)

2017–2020 **M.Sc. in Physics (GPA: 3.85; Academic Excellence Award)**, *Tribhuvan University*, Kathmandu, Nepal
Coursework: Computational Physics

2012–2016 **B.Sc. in Physics (68.8%)**, *Tribhuvan University*, Kathmandu, Nepal
Coursework: Material Science, Statistics, Linear Algebra

Research Experience

Jan 2025–Present **Project: Fine Tuning Large Language Models for Superconductor Discovery**, *University of New Hampshire*

- Built a large experimental superconductivity database containing **78,203 records** across **19,058 unique compositions** by extracting structured data from scientific literature using an **LLM-driven automated workflow**.
- Curated key superconducting descriptors including **chemical composition,** T_c**, pressure conditions, crystal/structural metadata, and critical fields**, enabling scalable downstream modeling and benchmarking.
- Fine-tuned multiple open-source LLMs (e.g., **Mistral, LLaMA, Qwen, Phi**) for supervised tasks such as **superconductor vs. non-superconductor classification** and T_c **regression** from composition-only and structure-informed inputs.
- Developed an **inverse-design framework** conditioned on target T_c to generate chemically plausible candidate superconductors, discovering **novel compositions** and enabling hypothesis generation via screening on external databases.

Jan 2024–Dec 2024 **Project: Machine Learning Models for Magnetic Materials Discovery**, *University of New Hampshire*

- Engineered features and trained classification models to distinguish nonmagnetic, ferromagnetic, and antiferromagnetic materials with 90% accuracy.
- Developed regression models to predict Curie and Néel transition temperatures for FM and AFM compounds.
- Identified 25 high-Curie-temperature ferromagnets and 13 antiferromagnets using model predictions.

Jan 2024–Present **Project: Northeast Materials Database (NEMAD)**, *University of New Hampshire*

- Enhanced GPTArticleExtractor to parse API-accessed articles, standard PDFs, scanned PDFs, and legacy handbooks, using advanced prompt engineering.
- Curated an open-access database of 67,573 magnetic, 19,195 superconducting, and 7,123 thermoelectric materials entries with both experimental and machine-extracted properties.
- Extracted experimentally verified material properties from literature to enable data-driven discovery of high-performance magnetic, superconducting, and thermoelectric compounds..

Jan 2023–Jan 2024 **Project: GPTArticleExtractor — Large-Scale Data Mining Pipeline**, *University of New Hampshire*

- Designed and implemented a scalable NLP pipeline using LLMs (OpenAI API + LangChain) to extract structured data from over 22,000 scientific articles.
- Integrated YOLOv8 for automated segmentation of figures, and text regions from scientific articles.
- Achieved 83% accuracy in automated information extraction, reducing manual annotation time by 90%.
- Developed a semantic vector embedding system to enable contextual material property search, improving retrieval accuracy by 45%.

Jan 2019–Dec 2020 **Project: Computational Study on Vibrational Properties of Metronidazole (M.Sc. Thesis)**, *Tribhuvan University*, Kathmandu, Nepal

- Performed **DFT** calculations of molecular geometry and vibrational spectra (IR/Raman) for Metronidazole isomers, validating computational results against experimental measurements.
- Analyzed vibrational frequencies of Metronidazole in ionic form, comparing C-13 labeled and unlabeled spectra in isolation and in Chloroform solvent..

Feb 2018–Aug 2018 **Project: Simulation Study of Electric Field Between Electrodes (M.Sc. Term Paper)**, *Tribhuvan University*, Kathmandu, Nepal

- Designed and analyzed electrostatic wiggler models with various electrode configurations using COMSOL Multiphysics, concluding that rectangular electrodes exhibit the highest electric field strength compared to semi-cylindrical and triangular configurations.

Teaching Experience

Summer 2023 **Co-Instructor of Record — Introduction to Physics**, *University of New Hampshire*, Durham, USA

- Co-led the design and delivery of the full curriculum for an undergraduate Introduction to Physics course (20+ students).
- Shared responsibilities for lecture instruction, lab supervision, grading, and student support.
- Prepared lecture materials, created assessments, and held office hours to support student learning.

2022–2025 **Teaching Assistant (multiple semesters)**, *University of New Hampshire*, Durham, USA

- Taught laboratory sections, set up experiments, and facilitated hands-on learning in introductory physics courses.
- Graded lab reports, homework assignments, and exams, providing timely and constructive feedback.
- Held regular office hours and offered one-on-one support to enhance student understanding.
- Collaborated with faculty to refine lab procedures and improve instructional materials.

Publications

2025 **Itani, S.**; Zhang, Y.; Itani, R.; Zang, J. *Large Language Models for Superconductor Discovery*. *arXiv preprint arXiv:2512.10847 (2025)*.

2024 **Itani, S.**; Zhang, Y.; Zang, J. *The Northeast Materials Database of Magnetic Materials*. *Nat Commun 16, 9415 (2025)*.

2025 **Itani, S.**; Zhang, Y.; Zang, J. *Large Language Model-Driven Database for Thermoelectric Materials*. *Computational Materials Science*, **253**, 113855.

2024 Zhang, Y.; **Itani, S.**; Khanal, K.; Okyere, E.; Smith, G.; Takahashi, K.; Zang, J. *GPTArticleExtractor: An Automated Workflow for Magnetic Material Database Construction*. *Journal of Magnetism and Magnetic Materials*, **597**, 172001.

2022 Jha, V.K.; Joshi, R.; Dhital, S.; Pangeni, N.; **Itani, S.**; Simkhada, R. *Computational Study on Electric Potential and Field within Differently Shaped Electrostatic Electrodes Pair*. In *Proceedings of the 6th International Conference on Advanced Engineering and ICT-Convergence (ICAEIC-2021)*, Seoul, Korea, 2021; Advanced Engineering and ICT-Convergence Proceedings (AEICP), Vol. 4, pp. 150–152; ISSN 2635-4586.

Conferences & Presentations

2025 **Oral**: *LLM-Driven Databases for Accelerating Discovery of Functional Materials,* Northeast Quantum Forum 2025: AI in Quantum October 14-17, 2025 Durham, New Hampshire.

2025 **Poster**: *LLM-Driven Databases for Accelerating Discovery of Functional Materials,* Northeast Quantum Forum 2025: AI in Quantum October 14-17, 2025 Durham, New Hampshire.

2025 **Poster**: *Northeast Materials Database (NEMAD): Enabling Discovery of High Transition Temperature Magnetic Compounds,* Annual Graduate Research Conference (GRC) at University of New Hampshire, Durham , NH.

2025 **Participant**:Joint March Meeting and April Meeting: Global Physics Summit, Anaheim, CA.

2025 **Oral**: *Comprehensive Machine Learning Framework to Identify Novel High-Performance Magnetic Compounds,* MMM-INTERMAG Joint Conference, New Orleans.

2024 **Poster**: *Northeast Materials Database (NEMAD)*. Northeast Quantum Forum, UNH.

2023 **Participant**, *IEEE Around-the-Clock Around-the-Globe Magnetics Conference*.

2020 **Workshop**, *Computational Technique and Superconductor for Ab-Initio Quantum Chemistry*, Kathmandu University.

2019 **Poster**, *National Symposium on Research, Development, and Innovation in Physics*, St. Xavier's College, Kathmandu.

2019 **Participant**, *Three-Week Experimental Training Program in Physics for International Students*, CHARUSAT, India.

Professional Service

2025 Peer reviewer for *Science and Technology of Advanced Materials: Methods*

Technical Skills

Machine Learning & AI
- **Frameworks & Libraries:** Scikit-learn, PyTorch, TensorFlow, LangChain, OpenAI API
- **Techniques & Models:** Deep Learning, Physics-Informed Neural Networks (PINNs), ResNets, Convolution Neural Network (CNN), Graph Neural Network (GNN), Large Language Models (LLMs), Prompt Engineering
- **High-Performance & Parallel:** High-Performance Computing (HPC), Slurm, MPI

Data Processing & Analysis
- **Languages & Packages:** Python (NumPy, Pandas), SQL
- **Tools:** Jupyter Notebook
- **Big Data:** Big Data Analytics

Data Visualization
- Matplotlib, Plotly, OriginLab,

Programming Languages
- Python, C, C++, SQL, HTML, CSS, JavaScript, LaTeX

Development Tools
- Git, GitHub, VS Code, Ubuntu

Scientific Software
- Gaussian, GaussView, COMSOL Multiphysics, Mathematica

Operating Systems
- Windows, Ubuntu, macOS

Honors & Awards

2022 The Bertram Husch Scholarship

2021 Fr. Marshall D. Moran Memorial Award for Academic Excellence (in M.Sc. Physics)

2019 First Prize, Poster Presentation, National Symposium on Research, Development, and Innovation in Physics, St. Xavier's College, Kathmandu

2019 First Prize, Creative Quiz, Science Manthan, CHARUSAT, Gujarat, India

Certifications & Licenses

2022 Responsible Conduct of Research and Scholarly Activity Certification, University of New Hampshire (required for incoming PhD students)

Professional Memberships

Member, American Physical Society (APS)
Member, IEEE Magnetics Society