AMRENDRA KUMAR TIWARI

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WORK EXPERIENCE

October 2024 – Current – Munich, Germany

Research Scholar – Department of Geo- and Environmental Sciences, LMU

❋ Working on "Thermal transport properties of lowermost mantle minerals - Insights from atomic-scale simulations".

January 2024 – September 2024 – Cologne, Germany

Research Scholar – Institute of Geology and Mineralogy, University of Cologne

❋ Working on "Thermal transport properties of lowermost mantle minerals - Insights from atomic-scale simulations".

March 2022 – December 2024 – Tamil Nadu, India

Research Intern – Simulation Center for Atomic and Nanoscale Materials (SCANMAT)

❋ A research paper on my Master's project "***High Capacity Hydrogen Storage Material Based on Transition Metal-based Complex hydrides NaMgTH6 (T=Sc-Cu) -an Ab-initio Study***" is under review for publication.

❋ Worked on Machine Learning models for predicting material properties and finding potential material for further analysis Using DFT/experiment.

❋ Trained and mentored internship students in VASP, QuantumEspresso, and VESTA software based on DFT for electronic structure calculations.

❋ Delivered a series of lectures on Hydrogen storage materials and Density Functional Theory (DFT) in weekly seminars at ScanMAT.

TECHNICAL SKILLS

First Principle Calculations

Working experience in electronic structure calculation using **Density Functional Theory (DFT)** tools like,

❋ **VASP** (Vienna Ab initio Simulation Package): Highly Proficient

- Extensive experience in performing electronic structure calculations using VASP.
- Proficient in setting up input files, defining appropriate parameters, and interpreting results.
- Skilled in analyzing and visualizing electronic properties and band structures.

- Demonstrated ability to model various materials and interfaces using VASP.

❋ **Quantum espresso**
❋ **Gaussian**
❋ **CASTEP**
❋ **PHONOPY**
❋ **Abinit Code**
❋ **MD Simulations**

Material Informatics

❋ Sufficient programming knowledge in **python.**
❋ Sufficient experience with **machine learning** libraries such as **TensorFlow, Keras, and Scikit-learn**.
❋ Sufficient knowledge in exploratory data analysis using **Pandas, seaborn, matplotlib, NumPy** etc.
❋ Sufficient knowledge in **data retrieval** in materials databases like **Materials project, ICSD, OQMD, Aflow** etc.
❋ Working experience in featuring materials using a **custom featuring code** and external features such as **matminer, pymatgen etc.**

Other Skills

Python — C/C++ — Linux — Latex — Microsoft Office — Java — Research — Data Analysis

Research Project (Ph.D.)

Thesis: "*Thermal transport properties of lowermost mantle minerals - Insights from atomic-scale simulations*"

Ludwig Maximilian University of Munich (10/2024 - Current)

The project investigates the thermal transport properties of minerals in the Earth's lower mantle through atomic-scale simulations. Focusing on lattice thermal conductivity under relevant conditions aims to shed light on heat flow dynamics across the core-mantle boundary, which is crucial for understanding the geodynamo and magnetic field reversals. Collaborating with other groups in mineral physics and experimental high-pressure mineral physics within the DeepDyn program, the research seeks to refine methodologies and contribute constraints to larger-scale geophysical models, fostering interdisciplinary collaboration and advancing our understanding of Earth's deep dynamics.

Project Supervisor: **Prof. Jahn Sandro**, LMU

Field of study: Geochemistry & Geophysics; Physics; Mineralogy Chemistry; Materials Science

Master Project

Thesis: "*High Capacity Hydrogen Storage Material Based on Transition Metal-based Complex Hydrides NaMgTH6 (T=Sc-Cu) -an Ab-initio Study*"

Thesis Google Drive Link

CENTRAL UNIVERSITY OF TAMILNADU (08/2022 - 06/2023)

My master project thesis explores the potential of NaMg*TM*H6 (where, *TM*=Sc to Cu) metal hydrides for hydrogen storage. Using VASP simulations, I predicted their crystal structure and investigated crucial properties like formation energy, hydrogen site energy, pDOS, charge density, ELF, COHP, Born, Bader, and Mullikan's charge analysis. The results indicate the materials' stability and their iono-covalent bonding behavior show promise for hydrogen storage applications in the hydrogen economy.

Project Supervisor: **Prof. P. Ravindran**, Central University of Tamilnadu

Field of study: Computational Condensed Matter Physics

Mini Summer Project

Project Report: *"A Preliminary Look To The Charged-Particles Distributions at Top **LHC** Energy Using PYTHIA Software"*

CENTRAL UNIVERSITY OF TAMILNADU (04/2022 - 07/2023)

The mini summer project aimed to investigate charged-particle distributions in p-p collisions at a center of mass energy of 13 TeV using the PYTHIA 8.3 Monte Carlo generator. This study is crucial for understanding global observables in p-p and heavy-ion collision experiments, providing insights into the nature of the phase transition from hadronic matter to partonic matter. By measuring higher-order cumulants of positive, negative, and net-charge particle distributions, the research contributes to the ongoing high luminosity program at the Large Hadron Collider (LHC) and establishes a baseline for future heavy-ion collision data analysis.

Project Supervisor: **Dr. Nirbhay Kumar Behera**, Assistant Professor, Central University of Tamilnadu

Six-Month French Certificate Course:

Course Duration: 6 Months

CENTRAL UNIVERSITY OF TAMILNADU (01/2022 - 06/2023)

I achieved an outstanding O Grade in a six-month French certificate course, where I gained basic proficiency in reading, writing, and speaking. This foundational knowledge has provided me with the skills to engage in various practical communication tasks in French.

Course Instructor: **Sushant Dubey**, Assistant Professor, Central University of Tamilnadu

EDUCATION

INTEGRATED MASTERS IN PHYSICS – 8.01 CGPA

Department of Physics, Central University of Tamil Nadu, Thiruvarur, Tamilnadu -2023

HIGHER SECONDARY – 87.6 %
Anil Saraswati Vidya Mandir, Ayodhya, CBSE-New Delhi -2018

HIGH SCHOOL – 9.6 CGPA
Anil Saraswati Vidya Mandir, Ayodhya, CBSE-New Delhi -2016

RESEARCH INTERESTS

✳ **Computational Mineral Physics:** My research interests lie in exploring the thermal transport properties of minerals in Earth's lower mantle through atomic-scale simulations, aiming to understand heat flow dynamics and their implications for the geodynamo and magnetic field reversals.

✳ **Hydrogen Storage Materials:** Investigation and design of hydrogen storage materials for efficient and safe hydrogen storage applications. Exploration of novel materials with high hydrogen storage capacity, desirable thermodynamics, and fast kinetics for hydrogen uptake and release.

Machine Learning models for predicting materials properties and finding potential material for further analysis using DFT/experiments.

SPECIAL INTERESTS

Research — Geology and Mineralogy — Solid State Physics — Materials designing — Featuring materials using atomic properties — Density functional theory — Machine Learning — Computational techniques — Computational Condensed Matter Physics — Data retrieving — VASP — Material Science — Computational Chemistry — Programming

PRESENTED & PARTICIPATED

✳ Presented poster in DeepDyn meeting, Rügen - November 2024

✳ Workshop on High-Pressure Mineral Physics and Magmatic Petrology, LMV Université Clermont Auvergne 04.11-08.11.2024

✳ Doctoral school on solid earth sciences, Les Houches France 30.9-11.10.2024

✳ Presented poster in GSGS Conference at University of Cologne - April 2024

✳ Eight-days workshop and conference in Evolution of Electronic Structure Theory & Experimental Realization - EESTER 2023

✳ One Month workshop in Quantum Information and Quantum Technology - 2023 (QIQT -2023)

✳ One-day Symposium in Non-Linear Dynamics- Dynamic Days of Delhi – XVI - 2022

❋ Four-day workshop in advancing industrial catalysis by synergy of experiments and supercomputing simulation – Bulgarian Academy of Sciences 2022

❋ Pacific Rim International Conference in Superconducting Materials: Fundamentals and Applications – PRISM 2022

❋ Participated in the International GeoGebra Conference, India, which was held online during 11-13 March, 2021

❋ Seven-day school in General relativity and cosmology – IUCAA-CUTN 2020

❋ Two-day workshop in Spectroscopy, Central University of Tamilnadu 2019

❋ Two-day Indo-Norway workshop on functional materials for energy technology (FMET-2019)

ACHIEVEMENTS

Extra-Curricular Achievements

❋ **Mentor** at Simulation Centre for Atomic and Nanoscale Materials (Scanmat)-Delivered a series of lectures at scanmat center in the field of material informatics.

❋ Participated in the District-level **Science Exhibition** on a working model in high school studies.

❋ Coordinated in organizing many festivals at the Central University of Tamilnadu.

❋ University-level badminton player.

LANGUAGE SKILLS

Mother tongue(s): **Hindi**
Other Language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken Production	Spoken interaction	
ENGLISH	C2	C2	B2	B2	C2
FRENCH	A1	B1	A1	A1	A1
GERMAN	A2	A2	A2	A2	A2

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

RECOMMENDATIONS

Prof. Jahn Sandro – Professor

Prof. Jahn Sandro

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Ludwig Maximilian University of Munich
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80333 Munich

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Prof. P.Ravindran – Professor

Prof. P. Ravindran
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Head, Simulation Center for Atomic and Nanoscale Materials (SCANMAT)
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Declaration:

I do hereby declare that all the above information provided by me is true to be the best of my knowledge and belief.