Kunwar Abhikeern

Research Scholar, IIT Bombay, India

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PROFILE SUMMARY

- Dedicated and adaptable researcher specializing in computational materials science, integrating molecular dynamics (MD), density functional theory (DFT) and machine learning (ML) techniques for materials discovery. Skilled in phonon dynamics, thermal transport analysis, and high-throughput simulations. Collaborative and solutions-driven, dedicated to advancing research.

ACADEMIC QUALIFICATIONS

- **PhD** *(2019 - 2024)*
  Mechanical Engineering, IIT Bombay, Mumbai, India *CGPA 8.71/10*
  Thesis: Lattice Thermal Conductivities and Phonon Properties of FPU based Lattices and Graphene with Layers, Grain Boundaries and Strain
  Supervisor: Prof. Amit Singh

- **Master of Technology** *(2015 - 2017)*
  Nanotechnology, IIT Roorkee, Roorkee, India *CGPA 7.2/10*
  Thesis: Efficient Numerical Methods for Solving Population Balance Models
  Supervisor: Prof. Ankik Giri

- **Bachelor of Technology** *(2010 - 2014)*
  Mechanical Engineering, Ajay Kumar Garg Engineering College, Ghaziabad, India *70.18%*
  Project: Reconfigurable Manufacturing System
  Supervisor: Prof. Pallab Biswas

RESEARCH INTERESTS

- Mathematical Modeling and simulation, Materials Discovery, Machine Learning for Materials Science, High-Throughput Materials Screening, Molecular Dynamics, Thermal Transport, Electronic Transport, Heat Transfer Modeling, Multiscale Simulations, Multiphysics modeling, Computational Chemistry, Coarse-Grained Modeling, Phonon Transport & Engineering

PROFESSIONAL EXPERIENCE

- **Research Associate** *(Nov 2024 - Present)*
  Mechanical Engineering, IIT Bombay, Mumbai, India
  - Developing ML-based interatomic potentials for $Mg_2Si_xSn_{1-x}$ thermoelectrics using the Spectral Neighbor Analysis Potential (SNAP) framework.
  - Training potentials on **DFT-calculated datasets** to achieve DFT-level accuracy while enabling computationally efficient simulations of larger systems and performing molecular dynamics (MD) simulations to study **thermal transport properties**.
  - Enhancing predictive models for **phonon interactions and lattice thermal conductivity**, contributing to the design of high-efficiency thermoelectric materials.
- **Materials Science Molecular Dynamics Software Developer - Intern** *(Feb 2024 - May 2024)*
  Schrödinger Inc., Hyderabad, India

- Developed a MD based numerical **local stress calculation driver**, an **atomistic scale modelling simulation** tool with an application - focused analysis of stress fields in polymers, alloys and disordered systems, having its application in semiconductor, battery, aerospace industry etc.
- Possess knowledge of developing Python-based **graphical user interfaces (GUI)** using tools like **Tkinter** for disseminating computational models to industry.

- **Teaching Faculty** *(March 2018 - Sep 2018)*
  KD Campus, New Delhi, India
  - Taught **Theory of Machines** & **Thermodynamics** to a class of 150 students, delivering structured lectures focused on fundamental concepts and problem-solving. Conducted interactive sessions, assessments, and doubt-clearing classes to enhance student understanding and exam preparation.

RESEARCH EXPERINCE

- Developing ML-based interatomic potentials for $Mg_2Si_xSn_{1-x}$ thermoelectrics using SNAP, trained on DFT calculations, achieving DFT-level accuracy while enabling faster simulations of larger systems, comparable to MD.
- Developing a machine learning interatomic potential for Si-Ge systems using DFT for structure optimization and SNAP potentials in LAMMPS to simulate 2D interfacial thermal transport.
- Performed computational analysis using MD-based Non-Equilibrium Molecular Dynamics (NEMD) and Spectral Energy Density (SED) techniques, achieving a consistent 65% reduction in lattice thermal conductivity (TC) of single-layer graphene (SLG) compared to twisted-bilayer graphene systems.
- Conducted the first detailed study using the SED technique on SLG with symmetric grain boundaries (GBs), reporting a 60% decrease in TC compared to pristine graphene.
- Investigated the effects of strain, curvature, and wrinkling on the thermal properties of SLG with GBs, comparing results from NEMD, Green-Kubo, and SED techniques.
- Utilized the SED method to calculate the thermal properties of the Fermi-Pasta-Ulam (FPU) model in regular polygonal 2D structures, providing insights into the anomalous thermal behavior of 2D materials.

RESEARCH PUBLICATIONS & CONFERENCES

- **Journals**
  - **Kunwar Abhikeern** and Amit Singh, "Lattice thermal conductivity and phonon properties of polycrystalline graphene", Nanoscale Adv., 7, 1125-1133, 2025
  - **Kunwar Abhikeern** and Amit Singh, "A consistent comparison of lattice thermal conductivities and phonon properties of single layer and bilayer graphene systems", *J. Appl. Phys.* 134, 224305, 2023
  - Abhishek Kumar, **Kunwar Abhikeern** and Amit Singh, "Decoupling the effects of ripples from tensile strain on the thermal conductivity of graphene and understanding the role of curvature on the thermal conductivity of graphene with grain boundaries" *(arXiv)*
  - **Kunwar Abhikeern** and Amit Singh, "FPU models: Study of its anomalous behaviour and thermal properties of 2D polygonal structures" *(manuscript submitted)*

- **Kunwar Abhikeern** and Aditya Roy, "Quantum-Accurate Machine Learning Interatomic Potentials for $Mg_2Si_xSn_{1-x} - Bi_2Te_ySe_{1-y}$ Thermoelectrics Using SNAP"*(under preparation)*
- **Kunwar Abhikeern**, Ashwani Kushwaha and Amit Singh, "Machine Learning Interatomic Potentials for 2D Interfacial Thermal Transport in Si-Ge Systems"*(under preparation)*
- **Meiksin, J., Abhikeern, K., Antimirova, E. et al.**, Materials Research Society celebrates 50th anniversary at 2023 MRS Spring Meeting & Exhibit. *MRS Bulletin*, 48 (9), 947-954

- **Conferences**
  - *Oral* and *Poster Presentation* titled Multiscale modeling of unsteady non-equilibrium Boltzmann transport equation with FEM, at 17^{th} U.S. National Congress on Computational Mechanics held in Albuquerque, New Mexico, USA, July 2023
  - *Poster Presentation* titled Multiscale modeling of unsteady non-equilibrium Boltzmann transport equation with FEM, at MRS Spring Conference, held in San Francisco, April 2023
  - *Oral Presentation* titled Study of Unsteady Thermal Transport in Single Layer Graphene with NMD approach at Thermoelectrics VCT, Japan organized virtually, 2020

TECHNICAL SKILLS

- **Programming Languages and Tools**: Python, MATLAB, AWK, C++, Bash
  - Developed a *local stress driver* for Schrödinger Inc.'s Materials Science Suite using **Python**, enabling efficient stress field calculations.
  - Implemented pre- and post-processing scripts to handle simulation data from **Quantum Espresso, LAMMPS, and GULP**, as well as solving complex nonlinear coupled differential equations using **Python, C++, and MATLAB**.
  - Proficient in **Bash** scripting for Linux-based system administration, workflow automation, and high-performance computing (HPC) job management.

- **Software:** Desmond, LAMMPS, GULP, Quantum Espresso, Phono3py
  - Conducted large-scale molecular dynamics (MD) simulations using **LAMMPS** to study thermal transport and mechanical properties of materials.
  - Performed lattice dynamics and phonon dispersion calculations with **GULP** and **Phono3py** to analyze vibrational properties and thermal conductivity.
  - Applied **Quantum Espresso** for first-principles density functional theory (DFT) calculations to investigate electronic and structural properties of materials.
  - Utilized **Desmond** for molecular simulations in computational chemistry and drug discovery, focusing on biomolecular interactions.

- **AI/ML-Based Software and Tools**: PyTorch, scikit-learn, Physics-Informed Neural Networks (PINNs)
  - Employed **PyTorch** and **scikit-learn** to develop machine learning interatomic potentials for **MgSi-BiTe** thermoelectric materials, improving efficiency in atomistic simulations.
  - Utilized **scikit-learn** for machine learning model development, data analysis, and predictive modeling.
  - Developed a **PINNs**-based model to study interfacial heat transfer, integrating physics constraints with deep learning.

- **Scientific Visualization Software**: Tkinter, Maestro, Ovito, VMD
  - Employed **Ovito** and **VMD** for high-quality visualization and analysis of molecular dynamics (MD) simulations, enabling in-depth structural and thermal transport studies.
  - Used **Maestro** for interactive molecular modeling and simulation setup in computational chemistry applications.
  - Developed custom **Tkinter**-based **GUI** visualization tools for interactive analysis of simulation data.
- **Other Skills**: GitHub,LaTeX, Computer-Aided Design (CAD), LabVIEW, Microsoft Office

TEACHING, INSTRUMENT HANDLING & OTHER SKILLS

- **Graduate Teaching Assistant** *(2019 - 2024)*
  Mechanical Engineering, IIT Bombay, Mumbai, India
  - *Measurement of Vibration of structures* | *Engineering Graphics & Drawing* | *Strength of Materials*
    Collaborated on experimental work, supervised over 200 students doing experiments and writing up professional laboratory reports; arranged weekly meetings to evaluate the students academic progress and help them prepare for exams. Proficient in AutoCAD & MATLAB for creating detailed diagrams, schematics and visualizations in technical projects.
- **Tools**
  - Vibration measurement using accelerometer/displacement sensor: Assisted in conducting experiments using sensors and LabVIEW software and evaluating undergraduate-level student reports

POSITIONS OF RESPONSIBILITY

- **PhD Placement Manager** *(2022 - 2023)*
  Institute Placement Team, IIT Bombay, Mumbai, India
  - Led a team of 15 members and successfully secured a record $\sim$40 % increase in placements for the on-campus PhD students during the tenure, highest across the country

COURSE WORK

- Introduction to modeling of materials from atomistics to continuum | Molecular Simulations for Materials Engineering |Introduction to Condensed Matter Physics |Finite Element and Boundary Element Methods | Mechanisms in Crystal Plasticity | Mechanics of Deformable Bodies| Mathematical Methods in Engineering

EXTRA-CURRICULAR ACTIVITIES

- Awarded with *"Color"* title for exceptional contributions across multiple sports during 2022-23 for Hostel 12, IIT Bombay
- Awarded as the *"Best Sportsperson"*, *SAKSHAM* Annual Sports Meet 2013-2014, AKGEC Ghaziabad

REFERENCES

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