Siddharth Karkhanis

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Professional Profile

Ph.D. researcher in physics specializing in computational modeling of soft condensed matter. Experienced in molecular simulations, parameter studies, and data-driven validation against experiments. Strong background in scientific programming (Python), Linux/HPC workflows, and technical communication; with prior training in electronic-structure and transport modeling of low-dimensional materials.

Education

Ph.D. in Physics **Houghton, USA**
Michigan Technological University *2021 – Present*

M.S. in Physics **Houghton, USA**
Michigan Technological University *2021 – 2023*

M.Sc. in Physics **Pune, India**
Savitribai Phule Pune University *2018 – 2020*

B.Sc. in Physics **Pune, India**
Savitribai Phule Pune University *2015 – 2018*

Research & Professional Experience

Ph.D. Researcher (Computational Soft Matter) **Houghton, USA**
Michigan Technological University *2021 – Present*

- Coarse-grained molecular dynamics studies of charged/dipolar fluids (e.g., ionic liquid-inspired models), focusing on dielectric and transport behavior.
- Designed reproducible simulation workflows (equilibration → sampling → parameter sweeps) and executed campaigns on Linux/HPC systems.
- Quantified structure and dynamics from equilibrium trajectories; performed sensitivity studies across model parameters (size/charge/dipole/short-range interactions).
- Conducted energetic/thermodynamic analyses including internal-energy decomposition and thermodynamic-integration style comparisons across model variants.

International Research Intern **Vienna, Austria**
ASC Austria (IAESTE / TU Wien) *2025*

- Built and validated simulation workflows for anisotropic particles (Gay–Berne ellipsoids), including data formats and Python-based generator scripts.
- Benchmarked isotropic reference systems and extended the framework toward charged/dipolar anisotropic models.
- Evaluated temperature/thermostat stability in rigid anisotropic systems with coupled translational/rotational degrees of freedom.

Researcher (Computational Condensed Matter) **Nashik, India**
Savitribai Phule Pune University *2018 – 2020*

- DFT-based studies of graphene and functionalized graphene: structural stability, electronic structure, and transport-relevant properties.
- Electronic transport / I–V analysis using first-principles workflows (SIESTA; transport analysis tools), including pseudopotential validation.

Teaching Experience

Graduate Teaching Assistant (Physics) **Houghton, USA**
Michigan Technological University *2021 – Present*

- Supported undergraduate physics through labs, recitations, grading, and office hours (conceptual + problem-solving focus).
- Mentored students and coordinated with course instructors on delivery and instructional materials.

Tutor / Instructor (Physics, Math, Programming) **Nashik, India**
Independent Instruction *2016 – 2020*

- One-on-one and small-group instruction emphasizing fundamentals, intuition-building, and exam preparation.

Selected Technical Projects

- **ML Classification: Fake Job Postings & User Response (Python):** Built a supervised learning pipeline with preprocessing, feature selection, and model comparison (decision tree, logistic regression, random forest, kNN, SVM).

- **Reaction Solver GUI for Particle Processes (Python / Tkinter):** Implemented a rule-based engine enforcing conservation laws to classify/validate particle reactions via an interactive GUI.
- **Quantum Mechanics Visualization Tool (MATLAB GUI):** Interactive computation and visualization of wavefunctions and probability densities for canonical model systems.

Selected Talks & Posters

- **APS March Meeting (2025)** — Poster: Coarse-grained simulations linking model parameters to viscosity and dielectric response.
- **APS March Meeting (2024)** — Oral: Dielectric response and electrostatic energetics from mean-field theory and simulations.
- **Raman Memorial Conference (2020)** — Poster: DFT-based study of functionalized graphene transport properties.

Technical Skills

- **Simulation & Modeling:** Molecular dynamics; coarse-grained modeling; Lennard–Jones / Stockmayer-type interactions; isotropic & anisotropic particle models; equilibrium trajectory analysis; transport/dielectric property estimation; model benchmarking vs experiments.
- **Programming & Computing:** Python (NumPy, Pandas, Matplotlib); Bash/shell scripting; MATLAB; basic C; reproducible workflows; Linux/HPC job execution.
- **Software:** LAMMPS; (familiar) GROMACS; SIESTA; GOLLUM; VMD, OVITO, VESTA, XCrySDen; GNUplot; LaTeX; GitHub (basic).

Honors & Awards

- **IAESTE International Research Internship Fellowship** — 2025
- **APS Travel Grant (MTU)** — 2024–2025
- **TIFR–NIUS Fellowship (Chemistry)** — 2016–2018
- **All-Rounder Student Award (HPT/RYK College)** — 2017–2018

References

Available upon request.