ANIKEYA ADITYA

Mons, BE • Work Authorization: Belgian Residence Permit (Unlimited Labor Market Access / **Marché du travail: Illimité**)

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Summary

Computational materials scientist with a Ph.D. in Materials Science and extensive experience in density functional theory (DFT), molecular dynamics (MD), and machine-learned force fields (MLFF). My research integrates atomistic simulations, graph neural networks, and scientific machine learning to enable structure-property prediction and AI-guided materials discovery. I have led first-author publications and developed scalable computational workflows for multiscale materials modeling in HPC environments.

Education

University of Southern California August 2019-Dec 2025
Ph.D, Materials Science

- Dissertation: Emergent Phenomena in Two-Dimensional Materials: A Molecular Dynamics and Machine Learning Investigation of Strain, Grain Boundaries, and Twisted Superlattices

University of Southern California May 2023-May 2025
M.S., Computer Science

University of Southern California August 2019-May 2025
M.S., Materials Engineering

University of California *Santa Cruz* September 2014-June 2018
B.S., Physics Highest Honors

- Thesis: Inferring the Mass Function of Primordial Black Holes From Gravitational Wave Observations

University of California *Santa Cruz* September 2014-June 2018
B.A., Mathematics Honors

Honors

- Graduate School Fellowship, USC, 2020
- Koret Undergraduate Research Scholarship, UCSC, 2017
- Ron Ruby Memorial Undergraduate Scholarship, UCSC, 2017
- Undergraduate Research Award, UCSC, 2017
- Chancellor's Undergraduate Internship Program Scholarship, UCSC, 2015
- Dean's Undergraduate Scholarship, UCSC, 2014
- UCSC First Year Honors Program, 2014

Publications

- **Aditya,A,** Irie, A, Dasgupta, N,et al. “Emerging Ferroelectric Domains: Stacking and Rotational Landscape of MoS2 Moiré Bilayers." ACS Nano. (In Press).
- Irie, A., **Aditya, A.**, Nomura, K., et al. (2024). "Thermoelectric Grain Boundary in Monolayer MoS2." The Journal of Physical Chemistry C. doi.org/10.1021/acs.jpcc.4c04339
- Baradwaj, N., **Aditya, A.**, Mishra, A., et al. (2024). "Probing phonon focusing, thermomechanical behavior, and moire patterns in van der Waals architectures using surface acoustic waves." npj 2D Materials and Applications. doi.org/10.1038/s41524-024-01315-5
- **Aditya, A.**, Mishra, A., Baradwaj, N., et al. (2023). "Wrinkles, Ridges, Miura-Ori, and Moire Patterns in MoSe2 Using Neural Networks." The Journal of Physical Chemistry Letters. doi.org/10.1021/acs.jpclett.2c03539
- Burns, K., Tan, A. M. Z., Hachtel, J. A., **Aditya, A.**, et al. (2023). "Tailoring the Angular Mismatch in MoS2 Homobilayers through Deformation Fields." Small. doi.org/10.1002/smll.202300098
- Linker, T., Nomura, K., **Aditya, A.**, et al. (2022). "Exploring Far-from-Equilibrium Ultrafast Polarization Control in Ferroelectric Oxides with Excited-State Neural Network Quantum Molecular Dynamics." Science Advances. doi.org/10.1126/sciadv.abk2625

- Rajak, P., **Aditya, A.**, Fukushima, S., et al. (2021). "Ex-NNQMD: Extreme-Scale Neural Network Quantum Molecular Dynamics." 2021 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW). doi.org/10.1109/ipdpsw52791.2021.00145

Research Experience

University of Southern California (USC) | Los Angeles, CA

Graduate Research Assistant | *Aug 2019 – Dec 2025*

- **Stacking & Rotational Landscape of Moiré Bilayers (2023 – 2025):**
  - Employed large-scale MD simulations to map moiré-domain formation in twisted MoS_2 bilayers, revealing how initial stacking order controls ferroelectric domain structure.
  - **Outcome:** *First-author publication in **ACS Nano** (2026).*
- **Machine Learning Interatomic Potential Development (2024 – Present):**
  - Developed and trained **NequIP-Allegro ML potentials** on *ab initio* MD datasets (VASP) to replicate DFT-level forces and energies in twisted perovskite moiré systems.
  - Validated models on unseen configurations, enabling high-throughput, nanosecond MD simulations of topological structures such as vortex/antivortex dynamics.
- **Multi-Layer Moiré Structure Generator (2025 – Present):**
  - Developed a Python-based computational toolkit for generating periodic multi-layer moiré supercells with arbitrary twist angles and stacking sequences across three or more layers.
  - Implemented vectorized geometric transformations and lattice symmetry operations to construct large commensurate supercells efficiently.
  - Optimized structure-generation routines using NumPy vectorization, Numba JIT compilation, and multiprocessing for scalable execution on HPC systems.
  - Designed the toolkit to generate the input structure to integrate seamlessly with VASP and LAMMPS workflows.
  - Code publicly available at **GitHub:** github.com/anikeya9/Multi-Layer-Moire-MLM- associated research software paper in preparation.
- **Thermodynamics of Grain-Boundary Interphases (2023 – 2024):**
  - Investigated a nanoscale interphase in monolayer MoS_2 using MD simulations.
  - **Outcome:** *Co-author publication in **The Journal of Physical Chemistry C** (2024).*
- **Wrinkles, Ridges, & Moiré Patterns in $MoSe_2$ (2021 – 2023):**
  - Investigated wrinkle-to-ridge transitions and ridge nucleation pathways under compression using MD simulations.
  - Mapped strain-induced 1T/2H superlattice formation through atomic-geometry analysis.
  - **Outcome:** *First-author publication in **The Journal of Physical Chemistry Letters** (2023).*

University of California, Santa Cruz (UCSC) | Santa Cruz, CA

Junior Specialist (Department of Chemistry) | *Aug 2018 – May 2019*

- **Domain-Specific Software Development:** Developed Python-based modules to estimate photoluminescence (PL) line shapes from defects in 2D materials.
- **Code Authorship:** Contributor to the **PL-lineshape-code** repository (Ping Group). GitHub: github.com/Ping-Group-UCSC/PL-lineshape-code
- **Electronic Structure Calculations:** Executed calculations in **Quantum ESPRESSO** to analyze band structure.

Undergraduate Researcher (Dept. of Physics) | *Sept 2016 – June 2018*

- **Computational Astrophysics (B.S. Thesis):** Developed a Bayesian Inference framework in **Mathematica** to infer the mass functions of Primordial Black Holes (PBH) from LIGO/Virgo gravitational wave data.
- **Statistical Modeling:** Extended monochromatic merger rate calculations to extended mass functions (Lognormal, Power-law) and implemented Bayesian tools to predict mass-function exponents from random binary merger samples.

Software Engineering & Applied Ml Projects

Beyond the Scoresheet: Soccer Analytics with Computer Vision

Team Lead | Aug 2024 – Dec 2024 | **GitHub:** github.com/anikeya9/bts-soccer-vision

- Led a 3-member team to design and deploy a CV pipeline using **YOLOv8** to detect and track players, ball, and referees.
- Integrated an **LSTM-based model** to predict trajectories and accurately impute missing positional data from occluded video feeds.

Parallel Analysis Tools for Large-Scale Simulations

GitHub: github.com/anikeya9/stacking-analysis

- Created custom parallel scripts (Numba, HPC) for post-processing massive MD trajectories(above 1B atoms), enabling rapid stacking identification across moiré configurations.

CUIP Intern (Cal Teach) | *Aug 2015 – June 2016*

- Redesigned a program database to enable granular data storage and on-demand reporting.
- Mined data to explore success trends in high-need schools, correlating outcomes with participant backgrounds.

Conference Presentations

- Aditya, A., et al. "Neural Network Dynamics for Barium Titanate (BaTiO3) Moire Structures" APS March Meeting, 2025
- Aditya, A., et al. "Controlling Ferroelectric Domains in Moire MoS ." APS March Meeting, 2024
- Aditya, A., et al. "Wrinkle Dynamics in Graphene Supported on a Polymer." IUPAP Conference on Computational Physics, 2022
- Aditya, A., et al. "Wrinkle Dynamics in Graphene Supported on a Polymer and Monolayer MoSe2 ." MRS Fall Meeting, 2022
- Aditya, A., et al. "Neural Network Molecular Dynamics of Ferroelectric Domain Boundary." APS March Meeting, 2021

Technical Skills

- Languages: Python (Numba, Multiprocessing), Mathematica, LaTeX, Shell Scripting.
- Machine Learning & AI: PyTorch, TensorFlow, Graph Neural Networks (GNNs), Equivariant Neural Networks based Interatomic Potentials (NequIP, Allegro), YOLOv8, LSTM, Bayesian Inference.
- Scientific Computing: LAMMPS, VASP, Quantum ESPRESSO, Molecular Dynamics (MD), Density Functional Theory (DFT).
- Software Engineering: Git, Linux/Unix, HPC Schedulers (SLURM), Parallel Computing, System Integration.
- Data & Visualization: Pandas, NumPy, SciPy, Matplotlib, Plotly, Seaborn.
- Workflow tools: ASE (Atomic Simulation Environment)
- Maintained public GitHub repository with documented examples, reproducible workflows, and version control practices.

Teaching Experience

Graduate Teaching Assistant | University of Southern California | *2019 – 2025*

- **Deep Learning (MASC-520):** Led tutorials on practical applications of deep learning in materials science and developed beginner-friendly Python tutorials.
- **Physics Laboratory:** Conducted lab sessions for Physics 135-A and 152-A, coordinating multiple sections and building student scientific skills.

Languages

- **English & Hindi:** C2 (Native/Bilingual Proficiency)
- **French:** Beginner (Currently learning; **resident in Wallonia, Belgium**)
- **Japanese:** Elementary