

ANIKEYA ADITYA

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Work Authorization: Belgian Residence Permit — *Marché du travail: Illimité (Unlimited EU Labor Market Access)*

SUMMARY

Multidisciplinary Computational Scientist and Applied Mathematician with 6+ years of research experience spanning molecular dynamics, density functional theory, machine-learned interatomic potentials, and applied deep learning. PhD in Materials Science (USC, 2025) with an MS in Computer Science and an MS in Materials Engineering. Three first-author publications in top ACS journals (ACS Nano, JPCL, JPCC). Expert at bridging deep mathematical theory — Bayesian inference, stochastic processes, differential equations — with high-performance software engineering (HPC, parallelized Python). Six years of self-directed research in distributed multi-institution collaborations (USC, Argonne, Florida, Sony); accustomed to async workflows and independent delivery without daily supervision. Seeking fully remote roles in computational science, AI/ML for science, data science, or sports analytics.

TECHNICAL SKILLS

Mathematical Modeling	Bayesian Inference, Monte Carlo Methods, Inverse Transform Sampling, ODE/PDE Solvers, Numerical Integration, Uncertainty Quantification, Statistical Signal Processing
Machine Learning & AI	Equivariant Neural Networks (NequIP, Allegro), Graph Neural Networks (GCN), CNNs (Transfer Learning), YOLOv8, LSTMs, UMAP, K-means Clustering; PyTorch, e3nn
Scientific Computing	Molecular Dynamics (LAMMPS), Density Functional Theory (VASP, Quantum ESPRESSO), ML Force Fields (MLIP), Non-Equilibrium MD, ASE
HPC & Performance	SLURM job scheduling, Numba JIT compilation, NumPy vectorization, Multiprocessing parallelization, Multi-GPU training, Linux systems
Software Engineering	Python (NumPy, SciPy, Pandas, PyTorch, Polars), Mathematica, Shell Scripting, Git/GitHub, Reproducible research workflows, VASP/LAMMPS I/O
Data & Visualization	Pandas, Matplotlib, Plotly, Seaborn; custom analysis pipelines for large-scale simulation data

SELECTED PUBLICATIONS

- Aditya et al. "Emerging Ferroelectric Domains: Stacking and Rotational Landscape of MoS₂ Moiré Bilayers." ACS Nano 2026, 20, 4702–4709. (First Author)
- Irie, Aditya et al. "Thermoelectric Grain Boundary in Monolayer MoS₂." J. Phys. Chem. C 2024, 128, 16172–16178. (Second Author)
- Aditya et al. "Wrinkles, Ridges, Miura-Ori, and Moiré Patterns in MoSe₂ Using Neural Networks." J. Phys. Chem. Lett. 2023, 14, 1732–1739. (First Author)
- 3 additional co-author publications in npj 2D Materials and Applications, Small, and Science Advances.

PROFESSIONAL EXPERIENCE

Computational Research Scientist (PhD Researcher)

Aug 2019 – Dec 2025

University of Southern California

- ML Force Field Development:** Designed, trained, and validated NequIP/Allegro equivariant neural network force fields on ab initio MD datasets (VASP/DFT). Achieved DFT-level accuracy (test RMSE: 3.88 meV/atom, 0.083 eV/Å)

forces) enabling nanosecond-scale MD simulations of systems up to 363,744 atoms — a scale inaccessible to direct DFT.

- **Scientific Software Engineering:** Architected MXM, a production-quality Python package for generating periodic multi-layer moiré supercells with arbitrary twist angles. Implemented Numba JIT-compiled kernels, NumPy vectorization, and multiprocessing parallelization (research software paper in preparation for Computer Physics Communications).
- **Deep Learning for Structural Analysis:** Trained CNNs with transfer learning (97% accuracy) to identify crystalline phases and defects in millions of atoms across large-scale MD trajectories. Applied to ferroelectric domain boundaries and strain-induced phase transitions in 2D materials.
- **Scalable HPC Workflows:** Engineered automated SLURM-based pipelines managing multi-TB datasets with post-processing scripts handling MD trajectories exceeding 1B atoms; achieved 10× throughput improvement via JIT and multiprocessing.
- **Applied Bayesian & Statistical Methods:** Developed potential energy surface analysis, dipole moment calculations, and stacking domain classifiers using atomic fingerprinting; quantified structural uncertainty across large configuration spaces.

Research Software Engineer (Junior Specialist)

Aug 2018 – May 2019

UC Santa Cruz — Ping Group

- Developed Python modules to compute photoluminescence lineshapes for NV-center point defects using DFT (Quantum ESPRESSO) + Fourier-transform generating function approach; code contributed to public Ping Group repository.
- Replaced numerically expensive integration routines with analytical expressions (Mathematica), significantly reducing CPU overhead while maintaining simulation fidelity.

Undergraduate Researcher — Applied Mathematics & Physics

Sept 2016 – June 2018

UC Santa Cruz

- Built a Bayesian inference framework to infer primordial black hole mass functions from LIGO/Virgo gravitational wave data; extended monochromatic merger rate calculations to lognormal and power-law extended mass functions.
- Implemented inverse transform sampling and Monte Carlo methods; validated against published results (Sasaki et al. 2016) using Dirac-delta limiting case.

KEY TECHNICAL PROJECTS

Soccer Analytics & Real-Time Tracking — Beyond the Scoresheet (BTS)

Aug–Dec 2024

- Led a 3-member team to build an end-to-end football video analysis pipeline: YOLOv8 fine-tuned for player/ball/referee detection (>90% mAP50); custom spatial-similarity multi-object tracker; SigLIP embeddings + UMAP (768D → 3D) + K-means for automated jersey-based team classification.
- Built a LSTM (8 frames → 4) for future trajectory forecasting; homography for bird's-eye pitch mapping.
- GitHub: github.com/anikeya9/bts-soccer-vision

MXM: Multi-Layer Moiré Structure Generator

- Engineered a high-performance Python library solving the hard problem of PBC-compatible supercell construction for 3+ twisted 2D material layers — a gap left by all existing bilayer-only tools.
- Production features: Numba @njit kernels, vectorized NumPy linear algebra, multiprocessing.Pool parallelization, Polars DataFrames, ASE I/O for VASP and LAMMPS. Research software paper in preparation.
- GitHub: github.com/anikeya9/Multi-Layer-Moire-MLM-

EDUCATION

Ph.D. in Materials Science — University of Southern California

Aug 2019 – Dec 2025

Dissertation: Emergent Phenomena in Two-Dimensional Materials: A MD and ML Investigation of Strain, Grain

Boundaries, and Twisted Superlattices

M.S. in Computer Science — *University of Southern California*

May 2023 – May 2025

M.S. in Materials Engineering — *University of Southern California*

Aug 2019 – May 2025

B.S. in Physics — Highest Honors | B.A. in Mathematics — Honors —
UC Santa Cruz

September 2014 – June 2018

*B.S. Thesis: Inferring the Mass Function of Primordial Black Holes from Gravitational Wave Observations (Advisor:
Prof. Stefano Profumo)*

LANGUAGES & INTERESTS

Languages: English & Hindi (C2, bilingual native); French (Beginner, living in Wallonia, Belgium); Japanese (Elementary).

Interests: Soccer analytics and sports data science; precision calligraphy and sketching; strategy and open-world gaming.

Work style: Highly experienced in asynchronous collaboration and distributed remote R&D teams; available for fully remote positions globally.

Full academic CV with complete publication list available on request • Last updated April 2026