Saurabh Sivakumar

sausiva@ucdavis.edu | LinkedIn | Github | Website | Google Scholar | +1 412 636 6213

Interests: *Multi-scale molecular simulations, Computational Chemistry and materials modelling, Geometric deep learning, Fine-tuning ML models, High-performance computing, Workflow automation*

Education

University of California — Davis, CA
Ph.D. *in Chemical Engineering* — ***Sep 2021 – Present***

Carnegie Mellon University — Pittsburgh, PA
M.S *in Chemical Engineering* — ***Aug 2019 – Dec 2020***
Thesis: *Applications of machine learning interatomic potentials in catalysis* — ***Advisor:*** *Zachary Ulissi*

National Institute of Technology — Tiruchirappalli, India
B.Tech *in Chemical Engineering, Minor in Economics* — ***Jul 2015 – May 2019***
Thesis: *Plant design for Trichloroethylene manufacturing* — ***Advisor:*** *S. Saravanan*

Skills

- **Languages:** Python, Bash, R, C++, LaTeX
- **Python Packages:** ASE, RDKit, Scipy, Pandas, Seaborn, Pymatgen, Pynta, RMG, VASP-kit, MDanalysis, OpenMM, CuPy, Numba, Parsl, Dask, Deap
- **Machine Learning:** PyTorch, scikit-learn, PyG, WandB
- **Technologies/Frameworks:** Git, Plotly, OpenAcc
- **Simulation Tools:** VASP, ORCA, QuantumEspresso, LAMMPS, PLUMED, Psi4, Gaussian, Zacros, PySCF, COMSOL, Cantera, OVITO, VMD

Publications

An Automated Pynta-based Curriculum for ML-Accelerated Calculation of Transition States
Trevor Price, ***Saurabh Sivakumar****, Matthew S. Johnson, Judit Zador and Ambarish Kulkarni*
[Paper Link]

Toward an ab Initio Description of Adsorbate Surface Dynamics
Saurabh Sivakumar *and Ambarish Kulkarni*
[Paper Link]

Cluster-MLP: An Active Learning Genetic Algorithm Framework for Accelerated Discovery of Global Minimum Configurations of Pure and Alloyed Nanoclusters
Rajesh K. Raju, ***Saurabh Sivakumar****, Xiaoxiao Wang and Zachary W Ulissi*
[Paper Link]

Enabling robust offline active learning for machine learning potentials using simple physics-based priors
Muhammed Shuaibi, ***Saurabh Sivakumar****, Rui Qi Chen and Zachary W Ulissi*
[Paper Link]

Experience

Graduate Researcher — Sep 2021 – Present
University of California — *Davis, CA*

- Working under the guidance of ***Ambarish Kulkarni*** on studying novel thermal and electro-catalysts for energy and chemical transformations.

Machine Learning Accelerated Catalysis and Materials Design

- Led ML-enabled simulation efforts for DOE and industry-funded projects on catalyst deactivation, electrochemical separations, and near surface gas phase reactions.

- Engineered machine-learned interatomic potentials(MLIPs) to model adsorption, diffusion, and reactions on catalytic surfaces—achieving up to 1000x speedups over density functional theory (DFT) and enabling mechanistic insights into reactions like methanol partial oxidation on silver and the reverse water-gas shift.
- Developed automated frameworks for transition state discovery and kinetic modeling by integrating graph and descriptor-based models with open-source Python libraries.
- Leveraged these MLIPs to simulate diverse catalytic and materials systems and support theory-experiment collaboration through advanced techniques including Microkinetic Modeling, Kinetic Monte Carlo, Metadynamics, and On-the-fly Probability Enhanced Sampling.
- Co-developed and deployed active learning pipelines for model training and data generation Code

Data-Driven Screening of Transition Metal (TM) Complexes for Oxygen Separation

- Designed and deployed high-throughput DFT workflows to screen transition metal complexes for O_2 binding, resulting in several candidate materials for electrochemical oxygen separation.
- Conducted thermodynamic analysis across oxidation states, identifying entropic effects as key drivers of O_2 binding behaviour in transition metal complexes.
- Benchmarked DFT functionals against coupled cluster methods (CCSD(T)) to evaluate accuracy and performance in property prediction.

Research Assistant Jan 2020 – Jul 2021

Carnegie Mellon University *Pittsburgh, PA*

Development of ML-Enhanced Frameworks for Atomistic Simulations

- Worked on an ARPA-E-funded project on surface segregation using deep reinforcement learning, focusing on dataset preparation and Bayesian hyperparameter optimization.
- Contributed to the development of open-source tools and sampling strategies to build an active learning framework leveraging physics-informed Behler-Parrinello Neural Networks to accelerate Nudged elastic band calculations and molecular dynamics. Code
- Built and validated software for global optimization of nanoclusters using a modified genetic algorithm enhanced with neural networks and Gaussian processes Code

Research Intern May 2018 – Aug 2018

Singapore University of Technology and Design *Singapore*

- Worked on building and studying lightweight solar PV modules with a poly-carbonate substitute under supervision of *Arief S Budiman*

Awards

NREL Kestrel compute grant Oct 2024 - Present

50,000+ node hrs

NSF ACCESS Discover and Maximize compute grants Oct 2021 - Jan 2025

8,000,000 Credits

Multiple NERSC compute grants Nov 2021 - Present

50,000+ CPU and GPU node hrs

Projects

- Extended the All-atom Diffusion Transformer (ADiT) with energy-aware fine-tuning, generating chemically valid, diverse 3D conformers on QM9 with state-of-the-art accuracy while reducing computational cost versus traditional ab initio sampling. Code
- Implemented and extended a multi-modal transformer (DOSTransformer) for predicting density of states in crystalline materials by adapting and enhancing existing open-source code, integrating structural and energy-level embeddings, prompt tuning, dynamic positional encoding, and benchmarking against GNN, MLP, and E(3)NN baselines. Code
- Accelerated the Chebyshev Interaction Model by porting code to GPU with OpenACC and optimizing performance using Nsight Compute profiling, enabling faster large-scale simulations. Code
- Applied ML techniques (NNs, k-NN, decision trees, logistic regression, PCA, t-SNE) to classification and time-series analysis, achieving $\geq$96% accuracy on the UC Irvine Musk dataset and uncovering trends in COVID-19 data from the New York Times. Code

Conferences & Posters/Talks

An Active Learning Framework for Accelerating Saddle Point Searches — Nov 2020
Presented at AIChE Annual Meeting 2020 [Poster Abstract Link] — *(Virtual)*

Developing integrated experiment-theory approaches for heterogeneous catalysis — April 2021
Presented at UC Davis - Sandia Symposium [Poster Link] — *Davis, CA*

Microkinetic modeling for integrated near surface gas phase kinetics — May 2022
Presented at CeRCAS Meeting 2022 — *San Francisco, CA*

Optimizing Chebyshev Interaction Model with Parallel Programming — Oct 2024
NERSC Annual User Group Meeting [Poster Link] — *Berkeley, CA*

Other professional activities

Judge, UC Davis Chemical Engineering symposium — *Sep 2023*

Teaching Assistant, Chemical Reaction Engineering — *Fall 2023*

Head, Media Relations – Pragyan (NITT's Technical Organization) — *Jan 2017 - Jul 2019*