JACOB JEFFRIES

Graduate Student

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SUMMARY

Ph.D. student in materials science and engineering focused on multi-scale modeling, high-performance computing, molecular dynamics, Monte Carlo methods, and applied physics.

SKILLS

Languages: Python, Julia, MATLAB, R, LaTeX, C++, C.

Packages: OVITO, PyTorch, NumPy, jax, Numba, pandas, polars, SQLALchemy, scipy

Softwares: LAMMPS, OVITO, VASP

PROJECTS

Python
Diffusion in rough potential energy landscapes
Analytical statistical mechanics and Kinetic Monte Carlo simulations to quantify diffusion on a rough potential energy surface.

LAMMPS Python
Chemical potential calculator — **github.com**
LAMMPS interface to calculate and fit chemical potentials of random solid solutions.

LAMMPS Python
Impurity concentration in concentrated alloys — **github.com/arXiv/PRM**
μpT pseudo-ensemble model for impurity concentration in concentrated alloys.

SciPy Python
Kinetic Monte Carlo crystal growth — **github.com/pypi**
Density functional theory-informed Kinetic Monte Carlo simulations of crystal growth of pentaerythritol tetranitrate and β-1,3,5,7-tetranitro-1,3,5,7-tetrazoctane.

PyTorch Python
Quadratic unconstrained binary optimization annealing — **github.com**
Metropolis annealing for solving the QUBO problem.

PyTorch Python
Portable cluster expansion fitting — **github.com**
Constrained cluster expansion fitting using PyTorch and cooper.

OVITO Python
Cowley short-range order parameter modifier — **github.com/pypi.org**
Custom OVITO modifier for calculating the Cowley short-range order parameter during a molecular dynamics run.

OVITO Python
Onsager coefficients calculator — **github.com/pypi.org**
Repository for calculating Onsager coefficients from a molecular dynamics run, including a general-purpose particle-reduction OVITO modifier.

SciPy Python
Optimal color palette generator — **github.com**
Color palette generator that maximizes pairwise CIELAB distance between colors in the palette.

EDUCATION

2023 -
Materials Science and Engineering (Ph.D.) — **Clemson University**
Computational multi-scale materials science for concentrated alloys, materials under extreme conditions, and nuclear materials. Focus on molecular dynamics and Monte Carlo methods.

2019 - 2022
Physics (B.S.), Magna Cum Laude — **Clemson University**
Minors in chemistry and mathematics, honors distinctions in physics and chemistry.

EXPERIENCE

2023 -
Graduate Research Assistant — **Department of Materials Science and Engineering, Clemson University**

- Atomistic simulations of concentrated alloys on high performance computers.
  - Molecular dynamics simulations of point-defect hopping.
  - Thermodynamics of point defects using molecular statics.
  - Molecular dynamics-informed phase-field simulations of radiation-induced segregation.
- Kinetic Monte Carlo simulations of vacancy hopping on rough potential energy surfaces.

2023 –
Graduate Student — **T1 Division, Los Alamos National Laboratory**

- GPU-accelerated Kinetic Monte Carlo simulations of organic crystal growth from solution using density functional tight binding bond energies on high-performance computers using PyTorch.
- GPU-accelerated quadratic unconstrained binary optimization for organic crystal equilibrium shapes using simulated annealing with PyTorch.

2022 – 2022 **Undergraduate Intern** **University of Maryland, College Park**

- Reservoir computing machine learning framework to predict national and state-level COVID-19 trends using the rescompy library.

2022 – 2022 **Undergraduate Researcher** **Department of Materials Science and Engineering, Clemson University**

- Non-equilibrium molecular dynamics simulations of vacancy hopping in tungsten on high-performance computers.
- Molecular dynamics simulations of point-defect hopping in iron-based concentrated alloys on high-performance computers.

2021 – 2022 **Undergraduate Researcher** **Department of Chemistry, Clemson University**

- Analysis of short-term chaos and long-term pseudo-random-number-generator-induced synchronization in the Langevin equation on rough potential energy surfaces.

2019 – 2022 **Undergraduate Researcher** **Department of Physics and Astronomy, Clemson University**

- Computational bioinformatics and protein thermodynamics on high-performance computers focused on targeted medicine.

PUBLICATIONS

[1] Mahesh Koirala, H. B. Mihiri Shashikala, Jacob Jeffries, Bohua Wu, Stacie K. Loftus, Jonathan H. Zippin, and Emil Alexov. Computational investigation of the pH dependence of stability of melanosome proteins: Implication for melanosome formation and disease. *International Journal of Molecular Sciences*, 22(15), 2021.

[2] Jacob Jeffries, Fadi Abdeljawad, Suveen Mathaudhu, Emmanuelle Marquis, and Enrique Martinez. Prediction of defect properties in concentrated solid solutions using a Langmuir-like model. *Phys. Rev. Mater.*, 9:033803, Mar 2025.

CONFERENCES

2021 *Virtual*
American Chemical Society Spring Virtual National Meeting
Oral presentation on instabilities of melanosome proteins (OCA2, SLC45A2, TYR, TPC2, and ATP7A) from point mutations and implication for disease

2024 *Kingston, Ontario*
The 16th conference of COmputer Simulation of IRradiation Effects in Solids
Oral presentation on diffusivity of vacancies on a noisy potential energy surface

2025 *Las Vegas, Nevada*
TMS 2025 Annual Meeting & Exhibition
Oral presentation on atomistic and statistical modeling of defect properties in concentrated solid solutions