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 R — **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**
μpT pseudo-ensemble model for impurity concentration in concentrated alloys.

PyTorch Python — **Kinetic Monte Carlo crystal growth** — **github.com**
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 and Enrique Martinez. Langmuir-like model of dilute impurities in concentrated solid solutions, 2024.

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