

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, Numba, pandas, scipy

Softwares: LAMMPS, OVITO

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 LAMMPS interface to calculate and fit chemical potentials of random solid solutions.	github.com
LAMMPS Python	Impurity concentration in concentrated alloys μpT pseudo-ensemble model for impurity concentration in concentrated alloys.	github.com/arXiv
PyTorch Python	Kinetic Monte Carlo crystal growth 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.	github.com
PyTorch Python	Quadratic unconstrained binary optimization annealing Metropolis annealing for solving the QUBO problem.	github.com
PyTorch Python	Portable cluster expansion fitting Constrained cluster expansion fitting using PyTorch and cooper.	github.com
OVITO Python	Cowley short-range order parameter modifier Custom OVITO modifier for calculating the Cowley short-range order parameter during a molecular dynamics run.	github.com/pypi.org
OVITO Python	Onsager coefficients calculator Repository for calculating Onsager coefficients from a molecular dynamics run, including a general-purpose particle-reduction OVITO modifier.	github.com/pypi.org
SciPy Python	Optimal color palette generator Color palette generator that maximizes pairwise CIELAB distance between colors in the palette.	github.com

EDUCATION

2023 -	Materials Science and Engineering (Ph.D.) Computational multi-scale materials science for concentrated alloys, materials under extreme conditions, and nuclear materials. Focus on molecular dynamics and Monte Carlo methods.	Clemson University
2019 - 2022	Physics (B.S.), Magna Cum Laude Minors in chemistry and mathematics, honors distinctions in physics and chemistry.	Clemson University

EXPERIENCE

2023 -	Graduate Research Assistant • Atomistic simulations of concentrated alloys on high performance computers. <ul style="list-style-type: none">– 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.	Department of Materials Science and Engineering, Clemson University
2023 -	Graduate Student • 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.	T1 Division, Los Alamos National Laboratory

2022 – 2022	Undergraduate Intern	University of Maryland, College Park
	<ul style="list-style-type: none"> • 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
	<ul style="list-style-type: none"> • 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
	<ul style="list-style-type: none"> • 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
	<ul style="list-style-type: none"> • Computational bioinformatics and protein thermodynamics on high-performance computers focused on targeted medicine. 	

PUBLICATIONS

References

- [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.