708-790-0915
Champaign
dpalmer3@illinois.edu

Daniel Palmer

GitHub:
https://github.com/dpalmer-anl
LinkedIn:
https://www.linkedin.com/in/daniel-palmer-6a8788170

Summary

I am a 5th year PhD student at the University of Illinois at Urbana Champaign for Materials Science, looking for research internships in computational materials science. I am interested in modeling of Condensed Matter Systems, Materials Data Informatics, Multi-scale Modeling and Uncertainty Quantification. I have 7+ years experience managing my own large software projects for various types of materials simulations. I have contributed to various open source software packages for Materials Science simulation and io, as well as published and contributed to articles published in academic journals.

Education

PhD, Materials Science and Engineering **August 2021 - June 2026 (expected)**
University of Illinois at Urbana-Champaign

- Digital Materials Fellowship

Bachelor of Science, Physics **August 2017 - May 2021**
University of Notre Dame

Research Experience

PhD Student in Dr. Harley Johnson's group **August 2021 - Current**

- Develop semi-empirical, multi-scale models to study relationship between structural and electronic properties of 2D Moiré materials.
- Develop uncertainty quantification methods to study uncertainty in models for 2D Moiré materials
- Participated in LLM for Materials Science Hackathon. Created an app to build CIF files from information gathered in experimental papers.

Science Undergraduate Laboratory Intern **May 2020 - August 2021**
Argonne National Laboratory *Lemont, Illinois*

- Created Python interface to calculate topological invariants of crystallographic data using Extended Huckel method and Z2pack python module. Can be used to screen for topologically non-trivial materials.
- Developed Python tools to publish computational materials datasets on the Materials Data Facility

Research Assistant **May 2019 - May 2021**
University of Notre Dame *Notre Dame, IN*

- Used molecular dynamics simulations to study thermotropic nematic Liquid Crystal systems

Publications

- Quantum Monte Carlo fitted total energy tight-binding model for twisted bilayer graphene by Daniel Palmer, Naheed Ferdous, Gabriel Brown, et al. *Submitted to Physical Review B, in review (2025)*
- Graphene-hBN interlayer interactions from Quantum Monte Carlo by Kittithat Krongchon, Tawfiqur Rakib, Daniel Palmer, et al. *Phys. Rev. B 112, 115130*
- Systematically Improvable Uncertainty Quantification Methods for Bilayer Graphene Multi-Scale Models by Daniel Palmer and Harley T. Johnson. (*in progress*)
- Graph Neural Network for Unified Electronic and Interatomic Potentials: Strain-tunable Electronic Structures in 2D Materials by Moon-ki Choi, Daniel Palmer, and Harley T. Johnson. (*in progress*)

Skills

Programming	Python, Matlab, Fortran ,C++, Git, LaTeX, Pytorch, JAX, Uncertainty Quantification, LangGraph, LangChain
Modeling	Density Functional Theory (DFT), Tight Binding (TB), Molecular Dynamics (MD) Neural Networks for interatomic MD potentials, Supervised and Unsupervised Learning