WILLIS O'LEARY

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EDUCATION

Massachusetts Institute of Technology (MIT) Cambridge, MA
PhD, Materials Science and Engineering, GPA 4.7/5.0 Expected Feb. 2024

- Thesis: Leveraging experiments and first-principles calculations to understand and tune metal exsolution in perovskites
- Visiting researcher at Technical University of Munich, Jan. 2022 – June 2023

California Institute of Technology (Caltech) Pasadena, CA
BS, Chemical Engineering (materials track), GPA 3.8/4.0 June 2018

- Visiting student at University of Cambridge (St. John's College), Fall 2017

SKILLS

Programming: Python (PyTorch, scikit-learn, numpy, scipy, matplotlib, Jupyter), C++, C, MATLAB, Scala, Ocaml.
Other computational: Bash shell scripting, *nix command line tools, High performance computing, Git.
Simulation Methods: Molecular dynamics, DFT, Force fields (classical, reactive, machine learning).
Chemistry Software: VASP, LAMMPS, Schrodinger (Jaguar, Maestro), CRYSTAL, VESTA, VMD.
Laboratory: Raman spectroscopy, Scanning electron microscopy, X-ray diffraction, Ceramic synthesis and processing.
Languages: English (native), German (conversational)

RELEVANT RESEARCH EXPERIENCE

Jennifer Rupp Group (Electrochemical Materials Laboratory), MIT Cambridge, MA
NSF Graduate Research Fellow Oct. 2018 – Feb. 2024

- Combined dozens of experiments and hundreds of quantum mechanical calculations to derive a quantitative physical model to understand and computationally design nanoparticle-decorated fuel cell electrocatalysts.
- Developed general method to characterize a material's local structure by merging experimental and simulated Raman spectra; leveraged machine learning force fields and linear response theory to reduce computational cost.
- Wrote and released Python software interfacing with quantum chemistry software to calculate Raman spectra; applied software to extract critical structural information from experimental Raman spectra of battery and fuel cell materials.
- Carried out quantum mechanical calculations as part of a collaboration to develop memristive chips for AI involving three departments and Ericsson; results upended hypothesized memristive mechanism and redirected research efforts.
- Established and led two successful international collaborations with computational materials scientists and physicists.
- Published work in well-respected journals; I expect 4 first-author publications and another 3-4 coauthor publications.

William Goddard Group, Caltech Pasadena, CA
Undergraduate Research Assistant Mar. 2016 – Sept. 2017

- Leveraged quantum mechanical calculations to derive 15-step mechanism for the catalytic formation of maleic anhydride on the surface of the vanadyl pyrophosphate catalyst; discovered that reaction required two material phases.
- Designed and implemented quantum mechanics/molecular mechanics (QM/MM) Python library interfacing with VASP and LAMMPS for application to liquid/solid interfaces and catalysis.

Laboratory for Reliable Software, NASA Jet Propulsion Laboratory (JPL) Pasadena, CA
Undergraduate Research Assistant June – Aug. 2015

- Developed novel code analysis software based on a non-relational database; wrote compiler plugins and scripts to process C source code; designed and wrote Ocaml API to form database queries and answer questions about the code.
- Demonstrated software's scalability to millions of lines of code by analyzing core software onboard the Curiosity rover and the Europa Clipper (launch date October 2024).
- Presented tool to core software engineers of Europa Clipper; components of the software are still in use at JPL.

HONORS AND AFFILIATIONS

NSF Graduate Research Fellowship (2019), Richard P. Schuster Memorial Prize (2018), George W. Green and Bernice E. Green Memorial Prize (2018), Tau Beta Pi (since 2018)