

WILLIS O'LEARY

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EDUCATION:

Massachusetts Institute of Technology

PhD student, Department of Materials Science and Engineering

Sept. 2018 – Present

California Institute of Technology

BS in Chemical Engineering (materials track), GPA 3.8/4.0

Sept. 2014 – June 2018

- Studied abroad at University of Cambridge (St. John's College) in Fall 2017

SKILLS:

- Laboratory:** Basic chemistry lab proficiency, UV-Vis, NMR, gas chromatography, atmospheric plasmas, Swagelok.
- Modelling:** Density functional theory, force fields, molecular dynamics, QM/MM.
- Programming:** C, Python, C++, Scala, Ocaml, Java, Bash, LaTeX, Mathematica, Matlab, Git.
- Chemistry software:** LAMMPS, ReaxFF, Jaguar, CRYSTAL, VASP, Maestro, VESTA, VMD, ChemDraw.
- Other software:** PBS, MS Office, macOS, MS Windows.

EXPERIENCE:

Electrochemical Materials Laboratory, MIT: Research Assistant

Oct. 2018 – present

- Studying perovskite-based catalysts for solar-driven thermochemical fuel production.

William Goddard Group, Caltech: Undergraduate Researcher

Mar. 2016 – Sept. 2017

- Modelled vanadyl pyrophosphate catalyst and discovered dual-phase atomistic mechanism.
- Designed and implemented QM/MM tool for modelling heterogeneous catalysts.
- Began work to model the mechanism of the oxygen evolution reaction on iridium dioxide.
- Periodically presented at group meeting, maintained scripts, and passed skills to other group members.

Laboratory for Reliable Software, NASA Jet Propulsion Laboratory: Undergraduate Researcher

June – Aug. 2015

- Wrote a new, database-driven tool to automate manual code analysis.
- Used the tool to analyze core software onboard the Curiosity rover and the future mission to Europa.
- Presented the tool to core software engineers of Europa mission.

Charles Wright Group, Portland State University: High School Intern

June – Aug. 2013, 2014

- Used symbolic execution to test an email server and to evaluate the technology's maturity.
- In collaboration with a team from MIT Lincoln Laboratory, extended KLEE, a symbolic execution tool, to find buffer overflows within C++ data structures.

Leslie Muldoon Group, Oregon Health & Science University: High School Intern

June – Aug. 2012

- Studied cancer killing abilities of chemotherapy-acetaminophen drug combo *in vitro*.
- Presented findings at state-level Intel science fair.
- Conducted several surgical procedures on rats and developed a simple graphical software program to aid in cell counting.

PUBLICATIONS:

O'Leary, W. C., Goddard, W. A., & Cheng, M. J. (2017). The Dual-Phase Mechanism for the Catalytic Conversion of n-Butane to Maleic Anhydride by the Vanadyl Pyrophosphate Heterogeneous Catalyst. *J. Phys. Chem. C* 121, 43, 24069-24076

HONORS AND AFFILIATIONS:

- 2019 National Science Foundation Graduate Research Fellowship
- 2018 Richard P. Schuster Memorial Prize
- 2018 George W. Green and Bernice E. Green Memorial Prize

- Tau Beta Pi member since 2018
- 2017 Cambridge Scholar (Study Abroad)
- 2017 Class of '52 60th Reunion Summer Undergraduate Research Fellow
- 2016 Prof. Fredrick H. Shair Summer Undergraduate Research Fellow
- 2015 Summer Undergraduate Research Fellow

SELECTED COURSEWORK:

Massachusetts Institute of Technology

Materials at Equilibrium (Classical and Statistical Thermodynamics)

Electrical, Optical, and Magnetic Properties of Materials (Quantum Mechanics and Solid State Physics)

California Institute of Technology

Introduction to Computer Programming

Introduction to Programming Methods

Computer Language Shop (Ocaml)

Decidability and Tractability

Calculus of One and Several Variables

Linear Algebra

Differential Equations

Intro. Methods of Applied Math for the Phys. Sciences

Classical Mechanics and Electromagnetism

Waves

General, Organic, and Physical Chemistry

Chemical Engineering Thermodynamics

Chemical Thermodynamics (graduate level)

Introduction to Statistical Thermodynamics (graduate level)

Introduction to Environmental Science and Engineering

Introduction to Chemical Engineering Computation

Transport Phenomena

Separation Processes

Dynamics and Control of Chemical Systems

Chemical Reaction Engineering

Electronic Materials Processing

Fundamentals of Sustainability Science and Engineering

Fundamentals of Materials Science

Experimental Methods in Solar Energy Conversion

Chemical Synthesis and Characterization for Chem. Eng.

Chem. Eng. Design Lab (Gold Nanoparticle Project)

Optimal Design of Chemical Systems

University of Cambridge

Polymer Chemistry

Inorganic Materials

Organic Solids

Energy Landscapes and Soft Materials

Solid Electrolytes

Computer Simulation Methods in Chemistry and Physics

OTHER INTERESTS:

- French language.
- Longboarding, cycling, swimming, rock climbing, and bodyweight conditioning.
- Backpacking and hiking.
- Cooking and baking.