

# 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:** Micropipetting, working in fume and bio hoods, cell culture, UV-Vis, NMR, atmospheric plasmas.
- In silico:** 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:

### William Goddard Group, California Institute of Technology: 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. The Journal of Physical Chemistry C.

## HONORS AND AFFILIATIONS:

- 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:

### 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.