

# WILLIS O'LEARY

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## EDUCATION:

### Massachusetts Institute of Technology

MS/PhD student in the Department of Materials Science & 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 St. John's College, University of Cambridge 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, Mac OSX, 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:

- 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)

### **University of Cambridge**

Polymer Chemistry  
Inorganic Materials  
Organic Solids

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

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.