# SUMMARY

PhD candidate with 3+ years of experience with computational chemical kinetics and open-source software development using Python and varied industry experience through the MIT Chemical Eng. Practice School and Georgia Tech co-op program.

# EDUCATION

| Massachusetts Institute of Technology, Cambridge, MA  | Anticipated Feb 2020 |
|---|----------------------|
| Ph.D. Chemical Engineering  | GPA: 4.8/5.0         |
| Massachusetts Institute of Technology, Cambridge, MA  | June 2017            |
| M.S. Chemical Engineering Practice  | GPA: 4.8/5.0         |
| – Received the William C. Rousseau Award in Leadership and Ethics in Chemical Engineering Pract | ice                  |
| Georgia Institute of Technology, Atlanta, GA  | May 2014             |
| B.S. Chemical and Biomolecular Engineering with Highest Honors                                  | GPA: 3.98/4.00       |

# WORK EXPERIENCE

#### **Graduate Research Assistant**

Massachusetts Institute of Technology, Department of Chemical Engineering, Cambridge, MA

- Advised by Prof. William Green, focusing on kinetic modeling of polycyclic aromatic hydrocarbon formation
- Lead developer of Reaction Mechanism Generator, an open-source program used by many industry and academic groups worldwide for automatically generating detailed reaction mechanisms
- Maintaining the RMG website, a Django site which allows users to directly access many RMG features
- Performing quantum chemistry calculations to determine thermochemical and kinetic parameters

#### **Practice School Consultant**

Woodside Energy, Perth, Western Australia, Australia

- Resolved mass balance discrepancies in high pressure fuel gas system via meter calibration and data reconciliation
- Designed and analyzed novel 3D printable heat exchanger designs using Solidworks and computational fluid dynamics

## Practice School Consultant

MedImmune, Gaithersburg, MD

- Developed software to simplify data analysis for hydrogen-deuterium exchange mass spectrometry
- Explored structure-property relationships of antibody solutions through experimental and computational methods

## **Undergraduate Research Assistant**

Georgia Institute of Technology, School of Chemical and Biomolecular Engineering, Atlanta, GA

- Worked in Prof. Yulin Deng's research group, focused on development of polyoxometalate based fuel cell
- Designed and constructed fuel cell assemblies with the aid of Autodesk Inventor

## **R&D Engineer Co-op**

Georgia Pacific Gypsum, Decatur, GA

- Investigated new formulations and lab-scale methods for improving wallboard and underlayment products
- Created preliminary designs for future pilot-scale production line at R&D facility

## SKILLS

Technical skills:

- Proficient: Microsoft Word/Excel/PowerPoint/Visio, Python, MATLAB, LaTeX, git, Mathematica, Aspen Plus, Q-Chem, Gaussian, CHEMKIN
- Some experience: Cython, Django, Pelican, Vim, Bash, Linux, HTML+CSS, COMSOL, Simulink, Solidworks

## Foreign languages:

Chinese (native speaker), French (basic proficiency)

Jan 2013 – Aug 2013

May 2015 – Present

Apr 2016 - May 2016

Feb 2016 - Mar 2016

May 2011 - Dec 2012

#### PUBLICATIONS

- Chu, T-C.; Buras, Z.; Oßwald, P.; Liu, M.; Goldman, M.; Green, W. H. Modeling of aromatics formation in fuel-rich methane oxy-combustion with an automatically generated pressure-dependent mechanism. *Phys. Chem. Chem. Phys.* Submitted.
- Liu, M.; Green, W. H. Capturing Aromaticity in Automatic Mechanism Generation. *Proc. Combust. Inst.* 2018, In Press.
- Lai, L.; Gudiyella, S.; Liu, M.; Green, W. H. Chemistry of Alkylaromatics Reconsidered. *Energy & Fuels* 2018, 32 (4), 5489–5500.
- Class, C. A.; Liu, M.; Vandeputte, A. G.; Green, W. H. Automatic Mechanism Generation for Pyrolysis of Di-Tert-Butyl Sulfide. *Phys. Chem. Chem. Phys.* 2016, *18*, 21651–21658.
- Liu, W.; Mu, W.; Liu, M.; Zhang, X.; Cai, H.; Deng, Y. Solar-Induced Direct Biomass-to-Electricity Hybrid Fuel Cell Using Polyoxometalates as Photocatalyst and Charge Carrier. *Nat. Commun.* 2014, *5*, 3208.

#### **PRESENTATIONS**

- **Liu, M.**; Green, W. H. Improved aromaticity handling and ring perception in RMG to model PAH formation. ACS National Meeting, Aug 2018.
- Liu, M.; Goldman, M. J.; Grinberg Dana, A.; Johnson, M. S.; Han, K.; Green, W. H. Advances in Predictive Kinetic Modeling Using Reaction Mechanism Generator. 37<sup>th</sup> International Symposium on Combustion, Aug 2018.
- Liu, M. Automated Reaction Mechanism Construction: Overview & Current Status. 4<sup>th</sup> International Workshop on Flame Chemistry. Jul 2018.
- Liu, M.; Han, K.; Green, W. H. Going bigger: Capturing PAH chemistry in RMG. 10<sup>th</sup> International Conference on Chemical Kinetics, May 2017.
- Liu, M.; Lai, L.; Carr, A.; Class, C.; Monrose, T.; Green, W. H. Supercritical Water Treatment of Alkyl Aromatics: Observations Beyond Model Predictions. AIChE Annual Meeting, Nov 2015.

#### **TEACHING EXPERIENCE**

# Graduate Teaching Assistant

Feb 2017 – Jun 2017

Massachusetts Institute of Technology, Department of Chemical Engineering, Cambridge, MA

- Led office hours and review sessions for helping students with homework and before exams
- Proctored and graded exams, and coordinated homework grading

#### Undergraduate Teaching Assistant

Georgia Institute of Technology, School of Mathematics, Atlanta, GA

- Taught recitation sessions of approx. 35 students twice a week per class, one to two classes per semester
- Wrote, proctored, and graded quizzes and exams, and held weekly office hours

#### **VOLUNTEERING AND ACTIVITIES**

- MIT Video Game Orchestra: Student-led group focused on arranging and performing music from various video games
- NetPals: Outreach program to connect with local middle schoolers about STEM fields via email exchanges
- MIT Archery Club and Georgia Tech Archery Club
- Georgia Tech Tau Beta Pi, Marketing Chair

Aug 2011 - May 2014