

## RESEARCHER · DEVELOPER

Seattle, WA

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# **Education**

## **University of Washington**

Seattle, WA

ADVISOR: PROF. XIAOSONG LI

Ph.D. IN CHEMISTRY

Sept. 2016-Current

GPA: 3.88

Walla Walla, WA

Whitman College
B.A. IN CHEMISTRY WITH HONORS, MINOR IN MATHEMATICS

Aug. 2012 - May 2016

ADVISOR: PROF. NATHAN E. BOLAND

GPA: 3.59

# **Honors & Awards**

2018 Honorable Mention, NSF GRFP

2017-2018 CEI Graduate Fellowship, University of Washington, Clean Energy Institute

2017-2018 DIRECT NSF NRT Traineeship, University of Washington, Clean Energy Institute

2017 **Graduate Fellowship**, Pacific Northwest National Lab

2016 **Exceptional Achievement in Chemistry**, Whitman College, Chemistry Dept.

2014-2015 Perry Research Grant, Whitman College

# **Publications**

- 4. Liu, H.; Jenkins, A.J.; **Wildman, A.**; Frisch, M.J.; Lipparini, F.; Mennucci, B.; Li, X. Time-Dependent Complete Active Space Embedded in a Polarizable Force Field. *J. Chem. Theory Comput.*, 2019, 15. DOI: 10.1021/acs.jctc.8b01152
- 3. **Wildman, A.**; Donati, G.; Lipparini, F.; Mennucci, B.; Li, X. Nonequilibrium Environment Dynamics in a Frequency-Dependent Polarizable Embedding Model, *J. Chem. Theory Comput.* 2018, 15. DOI: 10.1021/acs.jctc.8b00836
- 2. **Wildman, A.**; Martinez-Baez, E.; Clark, A.; Li, X. Anticorrelated contributions to pre-edge features of aluminate near-edge X-ray absorption spectroscopy in concentrated electrolytes, *J. Phys. Chem. Lett.*, 2018, 9. DOI: 10.1021/acs.jpclett.8b00642
- Donati, G.\*; Wildman, A.\*; Caprasecca, S; Lingerfelt, D.B.; Lipparini, F.; Mennucci, B.; Li, X., Coupling Real-Time Time Dependent Density Functional Theory with Polarizable Force Field, J. Phys. Chem. Lett., 2017, 8. DOI: 10.1021/acs.jpclett.7b02320.
   \*Co-First Authors

# **Presentations**

Mar. 2016 Wildman, A.; Boland, N.E. Oxalic Acid Influences Kinetics of Strong Chelate Exchange Reactions. 251st American Chemical Society National Meeting and Exposition.

San Diego, CA

Nov. 2015 **Wildman, A.**; Boland, N.E. Influence of Oxalic Acid on Rates of Ligand Exchange between Strong Chelating Agents. 24th Annual Murdock College Science Research Conference.

Vancouver, WA

Mar. 2015 Boland, N.E.; Stone A.T.; Nelson, T.; Harned, M.V.; Wildman, A. Adjunctive, Disjunctive and "Interjunctive"? Influence of ligand structure on kinetic pathways of ligand exchange. Abstracts of Papers, 249th American Chemical Society National Meeting.

Denver, CO

# **Outreach Activities**

## **Clean Energy Institute Ambassadors**

University of Washington

- Solar car derby at Thorton Creek Elementary, Martin Sortun Elementary, and Eastgate Elementary
- Solar car derby at Engineering Discovery Days
- Dye-sensitized solar cells at Ingraham High School

## **Research Computing Club**

University of Washington

- · RCC Vice President
- RCC mentorship program (Mentor)

#### **WC Science Outreach**

Whitman College

- Science night at Green Park Elementary
- Teaching the senses at Sharpstein Elementary

## **Chemistry Department**

Whitman College

- Served as undergraduate liason for visiting faculty hiring decision
- Tutored students from general, organic, and analytical chemistry courses

# **Research Interests**

## Modeling time dependent chemical enviroments

In condensed phase systems, the effects of the surrounding matrix are often non-negligible and time dependent. I aim to develop several low-scaling techniques to capture the time dependence of the environment as well as the system of interest.

## Multi-dimensional and non-linear spectroscopies

Multidimensional spectroscopies can give detailed information about electron and nuclear dynamics. Quantum chemical modeling can be vital in interpreting the spectra and the physical significance, since the dynamics can be explicitly modeled. I intend to apply real time TDDFT to complicated systems for which the spectral interpretation is not sufficient to understand the underlying dynamics.

# Data driven computational molecular science

With the increase in computational power and decrease in the cost of measurement in recent years, the amount of data availiable has increased dramatically. The field of computational molecular science is no exception. I plan to leverage this large amount of data to provide insights into complicated systems and to develop new, data-driven methods in the molecular realm to circumvent the traditional, yet computationally expensive techniques.

# **Teaching Experience**

## **University of Washington**

Seattle, WA

TEACHING ASSISTANT (GENERAL CHEMISTRY)

Sept. 2016 - Mar. 2017

#### **Whitman College**

Walla Walla, WA

TEACHING ASSISTANT (QUANTITATIVE ANALYSIS)

Sept. 2014 - Dec. 2015