

# Andrew Wildman

RESEARCHER · DEVELOPER

Seattle, WA

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## Summary

Driven computational researcher with a focus on creating scalable, performant, and user-friendly software. 7+ years of experience in chemical research with 5+ years of experience developing high-performance, distributed algorithms. Looking to work in a team to solve challenging computational problems and make those solutions accessible to non-experts.

## Education

### University of Washington

PH.D. IN CHEMISTRY

ADVISOR: PROF. XIAOSONG LI

THESIS: MODELING *Ab Initio* QUANTUM DYNAMICS IN COMPLEX SYSTEMS THROUGH MULTI-SCALE EMBEDDING

GPA: 3.88

Seattle, WA

Sept. 2016 - June 2021

### Whitman College

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

ADVISOR: PROF. NATHAN E. BOLAND

GPA: 3.59

Walla Walla, WA

Aug. 2012 - May 2016

## Skills

### Technical Communication

14 peer-reviewed publications, 5 conference presentations, 4 programming workshops

### Mentoring

Mentored 4 undergraduate and 6 graduate students

### DevOps

Expert: CI/CD, Linux administration.

### Programming

Expert: C++, Python, Git, CMake. Proficient: Rust, Fortran, LaTeX.

## Publications

15. Wildman, A.; Zhao, L.; Tao, Z.; Pavošević, F.; Hammes-Schiffer, S.; Li, X. Solvated Nuclear-Electronic Orbital Structure and Dynamics. *In Preparation*
14. Cruzeiro, V.W.D.; Wildman, A.; Li, X.; Paesani, F. Relationship between Hydrogen-Bonding Motifs and the 1b<sub>1</sub> Splitting in the X-Ray Emission Spectrum of Liquid Water. *The Journal of Physical Chemistry Letters*, 2021, 12. DOI: 10.1021/acs.jpclett.1c00486
13. Shelby, M.L.; Wildman, A.; Hayes, D.; Mara, M.W.; Lestrangle, P.J.; Cammarata, M.; Balducci, L.; Artamonov, M.; Lemke, H.T.; Zhu, D.; Seideman, T.; Hoffman, B.M.; Li, X.; Chen, L.X. Interplays of Electron and Nuclear Motions along CO Dissociation Trajectory in Myoglobin Revealed by Ultrafast X-Rays and Quantum Dynamics Calculations. *Proceedings of the National Academy of Sciences*, 2021, 118. DOI: 10.1073/pnas.2018966118
12. Zhao, L.; Wildman, A.; Pavošević, F.; Tully, J.C.; Hammes-Schiffer, S.; Li, X. Excited State Intramolecular Proton Transfer with Nuclear-Electronic Orbital Ehrenfest Dynamics *The Journal of Physical Chemistry Letters*, 2021, 12. DOI: 10.1021/acs.jpclett.1c00564
11. Grofe, A.; Zhao, R.; Wildman, A.; Stetina, T.F.; Li, X.; Bao, P.; Gao, J. Generalization of Block-Localized Wave Function for Constrained Optimization of Excited Determinants *The Journal of Chemical Theory and Computation*, 2020, 17. DOI: 10.1021/acs.jctc.0c01049
10. Zhao, L.; Wildman, A.; Tao, Z.; Schneider, P.; Hammes-Schiffer, S.; Li, X. Nuclear-Electronic Orbital Ehrenfest Dynamics *The Journal of Chemical Physics*, 2020, 153. DOI: 10.1063/5.0031019
9. Kuda-Singappulige, G.U.; Wildman, A.; Lingerfelt, D.B.; Li, X.; Aikens, C.M. Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene *The Journal of Physical Chemistry A*, 2020, 124. DOI: 10.1021/acs.jpca.0c09564
8. Lu, L.\*; Wildman, A.\*; Jenkins, A.J.; Young, L.; Clark, A.E.; Li, X. The “Hole” Story in Ionized Water from the Perspective of Ehrenfest Dynamics. *The Journal of Physical Chemistry Letters*, 2020, 11. DOI: 10.1021/acs.jpclett.0c02987

7. Zhao, L.; Tao, Z.; Pavošević, F.; **Wildman, A.**; Hammes-Schiffer, S.; Li, X. Real-Time Time-Dependent Nuclear-Electronic Orbital Approach: Dynamics beyond the Born-Oppenheimer Approximation. *The Journal of Physical Chemistry Letters*, 2020, 11. DOI: 10.1021/acs.jpclett.0c00701
  6. Williams-Young, D. B.; Petrone, A.; Sun, S.; Stetina, T. F.; Lestrangle, P.; Hoyer, C. E.; Nascimento, D. R.; Koulias, L. ; **Wildman, A.**; Kasper, J. M.; Goings, J. J.; Ding, F.; DePrince III, A. E.; Valeev, E. F.; Li, X. The Chronus Quantum (ChronusQ) Software Package. *WIREs Comput. Mol. Sci.*, 2019, 10. DOI: 10.1002/wcms.1436
  5. Clark, A. E.; Servis, M. J.; Liu, Z.; Martinez-Baez, E.; Su, J.; Batista, E. R.; Yang, P.; **Wildman, A.**; Stetina, T.; Li, X.; Newcomb, K.; Maginn, E. J.; Autschbach, J.; Dixon, D. A. Solvent Extraction through the Lens of Advanced Modeling and Simulation. *Ion Exchange and Solvent Extraction*, 2019, 23, Chapter 5. DOI: 10.1201/9781315114378
  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
  1. 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

## Honors & Awards

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- 2019 **Gudiksen, Paul H. and Karen S. Merit Fellowship**, University of Washington, Chemistry Dept.
- 2019 **Best Poster Award**, Northwest Theoretical and Computational Chemistry Conference
- 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

## Presentations

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| Sept. 2019 | <b>Wildman, A.</b> ; Cruzeiro, V.W.D.; Paesani, F.; Li, X. Origins of X-Ray Emission 1b <sub>1</sub> Splitting in Liquid Water. European Summer School for Quantum Chemistry  | Palermo, IT      |
| Jul. 2019  | <b>Wildman, A.</b> ; Dembowski, M.; Graham, T. R.; Martinez Baez, E.; Gorniak, R. M.; Pouvreau, M. J.; Prange, M.; Krzysko, A. J.; Zhang, X.; Semrouni, D.; Wang, H-W.; Li, X.; Schenter, G. K.; Rosso, K. M.; Pearce, C. I.; Clark, A. E.; Clark, S. B. Relating Structure to Spectroscopic Signatures. 2019 Energy Frontier Research Centers Principal Investigators' Meeting | Washington, D.C. |
| Jun. 2019  | <b>Wildman, A.</b> ; Paesani, F.; Li, X. Origins of Hydrogen-Bonding Driven X-Ray Emission Splitting in Liquid Water. Northwest Theoretical and Computational Chemistry Conference.   | Pullman, WA      |
| Mar. 2016  | <b>Wildman, A.</b> ; 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  | <b>Wildman, A.</b> ; 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    |

## Outreach Activities

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### Research Computing Club

*University of Washington*

- Hyak Governance Board Voting Representative (2020-2021)
- RCC President (2019-2020)
- RCC Vice President (2018-2019)
- RCC mentorship program [Mentor] (2017-2020)

### Clean Energy Institute Ambassadors

*University of Washington*

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

### WC Science Outreach

*Whitman College*

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