Joshua J. Goings, Ph.D.

Contact Information

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Education

Ph.D.	University of Washington, Seattle, WA	Theoretical Chemistry	2017
B.S.	Seattle Pacific University, Seattle, WA	Chemistry & Biochemistry	2012

Summary

Experienced researcher at the interface of chemistry, quantum computing, and machine learning. Recent highlights:

interpretable machine learning for molecular dynamics (publication #28)
reinforcement learning for accurate wave function compression (publication #31)
automated resource estimates for chemistry simulations on fault-tolerant quantum computers

Experience

Visiting Research Scientist — 07/2021 to present
Google Quantum AI via PRO Unlimited

Data Science Postdoctoral Research Fellow — 03/2021 to 07/2021
eScience Institute, University of Washington

Postdoctoral Research Associate — 07/2020 to 07/2021
University of Washington
Advisor: Prof. Xiaosong Li

Postdoctoral Research Associate — 08/2017 to 06/2020
Yale University (lab moved Jan 2018)
University of Illinois at Urbana-Champaign
Advisor: Prof. Sharon Hammes-Schiffer

Graduate Research Assistant — 07/2012 to 06/2017
NSF Graduate Research Fellow
University of Washington
Advisor: Prof. Xiaosong Li

Publications

31 **Reinforcement Learning Configuration Interaction**
J. J. Goings, H. Hu, C. Yang, and X. Li
J. Chem. Theory Comput., 2021, *17*, 5482–5491.

30 **Role of Intact Hydrogen-Bond Networks in Multiproton-Coupled Electron Transfer**
W. D. Guerra, E. Odella, M. Secor, J. J. Goings, M. N. Urrutia, B. L. Wadsworth, M. A. Gervaldo, L. E. Sereno, T. A. Moore, G. F. Moore, S. Hammes-Schiffer, A. L. Moore
J. Amer. Chem. Soc. 2020, *142*, 21842–21851.

29 **Formation of an Unusual Glutamine Tautomer in a Blue Light Using Flavin Photocycle Characterizes the Light-adapted State**
J. J. Goings, P. Li, Q. Zhu, S. Hammes-Schiffer
Proc. Natl. Acad. Sci. 2020, 117, 26626–26632.

28 **Nonequilibrium Dynamics of Proton-Coupled Electron Transfer in Proton Wires: Concerted but Asynchronous Mechanisms**
J. J. Goings, S. Hammes-Schiffer
ACS Cent. Sci. 2020, 6, 1594–1601.

27 **The Chronus Quantum Software Package**
D. B. Williams-Young, A. Petrone, S. Sun, T. F. Stetina, P. Lestrange, C. E. Hoyer, D. R. Nascimento, L. Koulias, A. Wildman, J. Kasper, J. J. Goings, F. Ding, A. E. DePrince III, E. F. Valeev, X. Li
WIREs Comput. Mol. Sci. 2020, e1436.

26 **Proton-Coupled Electron Transfer Across Benzimidazole Bridges in Bioinspired Proton Wires**
E. Odella[†], S. J. Mora[†], B. L. Wadsworth[†], J. J. Goings[†], M. A. Gervaldo, L. E. Sereno, T. L. Groy, D. Gust, T. A. Moore, G. F. Moore, S. Hammes-Schiffer, A. L. Moore
Chem. Sci. 2020, *11*, 3820–3828.
[†]Equal contribution.

25 **Early Photocycle of Slr1694 Blue-Light Using Flavin Photoreceptor Unraveled through Adiabatic Excited-State Quantum Mechanical/Molecular Mechanical Dynamics**
J. J. Goings, S. Hammes-Schiffer
J. Amer. Chem. Soc. 2019, *141*, 20470–20479.

24 **Proton-Coupled Electron Transfer Drives Long-Range Proton Translocation in Bioinspired Systems**
E. Odella[†], B. L. Wadsworth[†], S. J. Mora[†], J. J. Goings[†], M. T. Huynh, D. Gust, T. A. Moore, G. F. Moore, S. Hammes-Schiffer, A. L. Moore
J. Amer. Chem. Soc. 2019, *141*, 14057–14061.
[†]Equal contribution.

23 **Electron-Coupled Double Proton Transfer in the Slr1694 BLUF Photoreceptor: A Multireference Electronic Structure Study**
E. R. Sayfutyarova, J. J. Goings, S. Hammes-Schiffer
J. Phys. Chem. B. 2019, *123*, 439–447.

22 **Propensity for Proton Relay and Electrostatic Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor**
J. J. Goings, C. R. Reinhardt, S. Hammes-Schiffer
J. Amer. Chem. Soc. 2018, *140*, 15241–15251.

21 **Controlling Proton-Coupled Electron Transfer in Bio-Inspired Artificial Photosynthetic Relays**
E. Odella, S. J. Mora, B. L. Wadsworth, M. T. Huynh, J. J. Goings, P. A. Liddell, T. L. Groy, M. Gervaldo, L. E. Sereno, D. Gust, T. A. Moore, G. F. Moore, S. Hammes-Schiffer, A. L. Moore
J. Amer. Chem. Soc. 2018, *140*, 15450–15460.

20 **Orientation-Dependent Imaging of Electronically Excited Quantum Dots***
D. Nguyen, J. J. Goings, H. A. Nguyen, J. Lyding X. Li, M. Gruebele
J. Chem. Phys., 2018, *148*, 064701.
**2018 JCP Editors' Choice*

19 **Current Development of Noncollinear Electronic Structure Theory**
J. J. Goings, F. Egidi, X. Li
Int. J. Quantum Chem. 2018, *118*, e25398.

18 **Real-Time Time-Dependent Electronic Structure Theory**
J. J. Goings, P. J. Lestrange, X. Li
WIREs Comput. Mol. Sci. 2017, e1341.

17 **Two-Component Non-Collinear Time-Dependent Spin Density Functional Theory for Excited State Calculations**
F. Egidi, S. Sun, J. J. Goings, G. Scalmani, M. J. Frisch, X. Li
J. Chem. Theory Comput. 2017, *13*, 2591–2603.

16 **Can Quantized Vibrational Effects Be Obtained from Ehrenfest Mixed Quantum-Classical Dynamics?**
J. J. Goings, D. B. Lingerfelt, X. Li
J. Phys. Chem. Lett. 2016, *7*, 5193–5197.

15 **Accelerating Real-Time Time-Dependent Density Functional Theory with a Non-Recursive Chebyshev Expansion of the Quantum Propagator**
D. Williams-Young, J. J. Goings, X. Li
J. Chem. Theory Comput. 2016, *12*, 5333–5338.

14 **Quantum Confinement Effects on Optical Transitions in Nanodiamonds Containing Nitrogen Vacancies**
A. Petrone, J. J. Goings, X. Li
Phys. Rev. B. 2016, *94*, 165402.

13 **Real Time Propagation of the Exact Two Component Time-Dependent Density Functional Theory**
J. J. Goings, J. M. Kasper, F. Egidi, S. Sun, X. Li
J. Chem. Phys. 2016, *145*, 104107.

12 **A Direct Atomic-Orbital Based Relativistic Two-Component Linear Response Method for Calculating Excited State Fine Structures**
F. Egidi, J. J. Goings, M. J. Frisch, X. Li
J. Chem. Theory Comput. 2016, *12*, 3711–3718.

11 **An Atomic Orbital Based Real-Time Time-Dependent Density Functional Theory for Computing Electronic Circular Dichroism Band Spectra**
J. J. Goings, X. Li
J. Chem. Phys. 2016, *144*, 234102.

10 **Imaging Excited Orbitals of Quantum Dots: Experiment and Electronic Structure Theory**
L. Nienhaus[†], J. J. Goings[†], D. Nguyen, S. Wieghold, J. Lyding, X. Li, M. Gruebele
J. Amer. Chem. Soc. 2015, *137*, 14743–14750.
[†]Equal contribution.

9 **Approximate Singly Excited States from a Two-Component Hartree-Fock Reference**
J. J. Goings, F. Ding, E. R. Davidson, X. Li
J. Chem. Phys. 2015, *143*, 144106.

8 **Ab Initio Two-Component Ehrenfest Dynamics**
F. Ding, J. J. Goings, H. Liu, D. Lingerfelt, X. Li
J. Chem. Phys. 2015, *143*, 114105.

7 **Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-Edge X-ray Absorption Spectroscopy**
B. Peng, P. J. Lestrange, J. J. Goings, M. Caricato, X. Li
J. Chem. Theory Comput. 2015, *11*, 4146–4153.

6 **Stability of the Complex Generalized Hartree-Fock Equations**
J. J. Goings, F. Ding., M. J. Frisch, X. Li
J. Chem. Phys. 2015, *142*, 154109.

5 **Ab Initio Non-Relativistic Spin Dynamics**
F. Ding, J. J. Goings, M. J. Frisch, X. Li
J. Chem. Phys. 2014, *141*, 214111.

4 **Theoretical Characterization of Conduction-Band Electrons in Photodoped and Aluminum-Doped Zinc Oxide (AZO) Quantum Dots**
J. J. Goings, A. M. Schimpf, J. W. May, R. W. Johns, D. R. Gamelin, X. Li
J. Phys. Chem. C. 2014, *118*, 26584–26590.

3 **Assessment of Low-Scaling Approximations to the Equation of Motion Coupled-Cluster Singles and Doubles Equations**
J. J. Goings, M. Caricato, M. Frisch, X. Li
J. Chem. Phys. 2014, *141*, 164116.

2 **Sorption of H_2 to Open Metal Sites in a Metal Organic Framework: A Symmetry Adapted Perturbation Analysis**
J. J. Goings, S. Ohlsen, K. Blaisdell, D. Schofield
J. Phys. Chem. A. 2014, *118*, 7411–7417.

1 **Self-Consistent-Field Using Direct Inversion in Iterative Subspace Method and Quasi-Newton Vectors**
J. J. Goings, F. Ding, X. Li
Adv. Quantum Chem. 2014, *68*, 77–86.

Awards

University of Washington Data Science Postdoctoral Fellow	2021
Chemical Computing Group (CCG) Excellence Award	2016
National Science Foundation (NSF) Graduate Research Fellow	2014
Bernard and Claudine Nist Endowed Fellowship in Chemistry	2014
Peter Salamon Award, Telluride Science Research Center	2014
Natt-Lingafelter Graduate Fellowship Award	2012
David T. & Christina L. Wong Scholarship in Chemistry	2011

Oral Presentations

- *Impact of protein conformational changes and electrostatics on a BLUF photoreceptor.*
  258th ACS National Meeting, San Diego, CA (2019)
- *Engineering a redox-active proton wire with proton-coupled electron transfer.*
  258th ACS National Meeting, San Diego, CA (2019)
- *Can quantized vibrational effects be obtained from Ehrenfest mixed quantum-classical dynamics?*
  253rd ACS National Meeting, San Francisco, CA (2017)
- *Atomic-orbital based real-time TDDFT for circular dichroism spectroscopy.*
  251st ACS National Meeting, San Diego, CA (2016)
- *Theoretical investigation of magnetic exchange interactions in dilute magnetic semiconductor quantum dots induced by defects.*
  Pacifichem 2015, Honolulu, HI (2015)
- *Linear Response Complex Generalized Hartree-Fock.*
  249th ACS National Meeting, Denver, CO (2015)
- *Equation of motion formalism of second order many-body perturbation theory (EOM-MBPT2) and second-order approximate coupled-cluster (CC2).*
  248th ACS National Meeting, San Francisco, CA (2014)
- *Low-Scaling Approximations to the Equation of Motion Coupled-Cluster Singles and Doubles Equations.*
  Excited States and Time-Dependent Electronic Structure Theory, Telluride, CO (2014)

Poster Presentations

- *Propensity for Proton Relay and Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor.*
  Gordon Research Conference on Computational Chemistry, West Dover, VT (2018)
- *Real Time Propagation of the Exact Relativistic Two-Component Equations.*
  Theory and Applications of Computational Chemistry (TACC), Seattle, WA (2016)
- *Recent advances in real-time TDDFT for the description of optical activity.*
  Low-scaling and Unconventional Electronic Structure Techniques Conference (LUEST), Telluride, CO (2016)
- *Towards a Real-Time Description of Magnetic Systems with Applications to Magnetic Circular Dichroism Spectroscopy.*
  251st ACS National Meeting, San Diego, CA (2016)

Teaching

Lecturer, Chemistry, University of Washington — Winter 2021
CHEM 465/565: Computational Chemistry
- Lead instructor; re-designed course for asynchronous online learning.
- Managed team of TAs to facilitate hands-on student experience with modern computational chemistry software and UW's high-performance computing (HPC) resources.
- Lectures highlighted fundamental and recent developments in computational chemistry.
- Guided students in novel research projects utilizing state-of-the art methods and computing resources directly applicable to individual research interests.

Teaching Assistant, Chemistry, Yale University — Spring 2019
CHEM 426/526: Computational Chemistry and Biochemistry
- Designed a computational chemistry course for graduate and undergraduate students.
- Gave students hands-on guidance using computational chemistry software.
- Facilitated student access to Yale's high-performance computing center.
- Performed computational "demos" at the end of each lecture; guest lectured as necessary.

Guest Lecturer, Chemistry, Seattle Pacific University — Spring 2016
CHM 2960: Introduction to Research Methods
- Lecture title: "Molecules and Light (or, Why you see what you see)."
- Introduction to computational spectroscopy for undergraduate chemistry majors.

Guest Lecturer, Chemistry, Seattle Pacific University — Spring 2015
CHM 2960: Introduction to Research Methods
- Lecture title: "Explorations into Molecular Magnetism."
- Introduction to computational chemistry research with undergraduate chemistry majors.

Teaching Assistant, Chemistry, University of Washington — Spring 2014
CHEM 465/565 Computational Chemistry
- Gave students hands-on guidance using computational chemistry software.
- Guided groups to perform novel computational research projects.

Teaching Assistant, Chemistry, University of Washington — Summer 2013
CHEM 162 General Chemistry
- Taught lab and quiz section to undergraduates.

Teaching Assistant, Chemistry, University of Washington — Winter 2013
CHEM 152: General Chemistry
- Taught two lab and two quiz sections to undergraduates.

Teaching Assistant, Chemistry, University of Washington — Autumn 2012
CHEM 142: General Chemistry
- Taught two lab and two quiz sections to undergraduates.