

Joshua Goings | Curriculum Vitae

Yale University, Department of Chemistry
225 Prospect St, New Haven, CT 06511

✉ josh [dot] goings [at] yale [dot] edu • 🌐 joshuagoings.com

Last Updated: December 20, 2018

Education

PhD Theoretical Chemistry

Advisor: Prof. Xiaosong Li

University of Washington

June 2017

BS Chemistry & Biochemistry

Summa Cum Laude

Seattle Pacific University

June 2012

Professional Experience

Postdoctoral Research Associate

Advisor: Prof. Sharon Hammes-Schiffer

Yale University

April 2018 – present

University of Illinois

August 2017 – April 2018

Postdoctoral Research Associate

Advisor: Prof. Xiaosong Li

University of Washington

June 2017 – August 2017

Honors and Awards

2016: Chemical Computing Group (CCG) Excellence Award

2014: National Science Foundation (NSF) Graduate Research Fellow

2014: Bernard and Claudine Nist Endowed Fellowship in Chemistry

2014: Peter Salamon Award, Telluride Science Research Center

2012: Natt-Lingafelter Graduate Fellowship Award

2010: NSF Research Experience for Undergraduates (REU) Fellow

(with Prof. Michael B. Smith, Univ. of Connecticut.)

Publications

(23): E. R. Sayfutyarova, **J. J. Goings**, S. Hammes-Schiffer, "Electron-Coupled Double Proton Transfer in the Slr1694 BLUF Photoreceptor: A Multireference Electronic Structure Study," *J. Phys. Chem. B*, 2018, *Just Accepted*.

(22): 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, "Controlling Proton-Coupled Electron Transfer in Bio-Inspired Artificial Photosynthetic Relays," *J. Amer. Chem. Soc.*, 2018, 140 (45), 15450–15460.

- (21): **J. J. Goings**, C. R. Reinhardt, S. Hammes-Schiffer, "Propensity for Proton Relay and Electrostatic Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor," *J. Amer. Chem. Soc.*, 2018, 140 (45), 15241–15251.
- (20): D. Nguyen, **J. J. Goings**, H. A. Nguyen, J. Lyding X. Li, M. Gruebele, "Orientation-dependent imaging of electronically excited quantum dots," *J. Chem. Phys.*, 2018, 148 (6), 064701.
- (19): **J. J. Goings**, P. J. Lestrangle, X. Li, "Real-Time Time-Dependent Electronic Structure Theory," *WIREs Comput. Mol. Sci.*, 2017, e1341.
- (18): F. Egidi, S. Sun, **J. J. Goings**, G. Scalmani, M. J. Frisch, X. Li, "Two-Component Non-Collinear Time-Dependent Spin Density Functional Theory for Excited State Calculations," *J. Chem. Theory Comput.*, 2017, 13 (6), 2591–2603.
- (17): **J. J. Goings**, F. Egidi, X. Li, "Current Development of Noncollinear Electronic Structure Theory," *Int. J. Quantum Chem.*, 2017;00:e25398.
- (16): **J. J. Goings**, D. B. Lingerfelt, X. Li, "Can Quantized Vibrational Effects Be Obtained from Ehrenfest Mixed Quantum-Classical Dynamics?" *J. Phys. Chem. Lett.*, 2016, 7, 5193–5197.
- (15): D. Williams-Young, **J. J. Goings**, X. Li, "Accelerating Real-Time Time-Dependent Density Functional Theory with a Non-Recursive Chebyshev Expansion of the Quantum Propagator," *J. Chem. Theory Comput.*, 2016, 12 (11), 5333–5338.
- (14): A. Petrone, **J. J. Goings**, X. Li, "Quantum Confinement Effects on Optical Transitions in Nanodiamonds Containing Nitrogen Vacancies," *Phys. Rev. B*, 2016, 94 (16), 165402.
- (13): **J. J. Goings**, J. M. Kasper, F. Egidi, S. Sun, X. Li, "Real Time Propagation of the Exact Two Component Time-Dependent Density Functional Theory," *J. Chem. Phys.* 2016, 145 (10), 104107.
- (12): F. Egidi, **J. J. Goings**, M. J. Frisch, X. Li, "A Direct Atomic-Orbital Based Relativistic Two-Component Linear Response Method for Calculating Excited State Fine Structures," *J. Chem. Theory Comput.* 2016, 12 (8), 3711–3718.
- (11): **J. J. Goings**, X. Li, "An Atomic Orbital Based Real-Time Time-Dependent Density Functional Theory for Computing Electronic Circular Dichroism Band Spectra," *J. Chem. Phys.* 2016, 144 (23), 234102.
- (10): L. Nienhaus*, **J. J. Goings***, D. Nguyen, S. Wieghold, J. Lyding, X. Li, M. Gruebele, "Imaging Excited Orbitals of Quantum Dots: Experiment and Electronic Structure Theory", *J. Amer. Chem. Soc.* 2015, 137 (46), 14743–14750. *Authors contributed equally to work
- (9): **J. J. Goings**, F. Ding, E. R. Davidson, X. Li, "Approximate Singly Excited States from a Two-Component Hartree-Fock Reference," *J. Chem. Phys.* 2015, 143 (14), 144106.
- (8): F. Ding, **J. J. Goings**, H. Liu, D. Lingerfelt, X. Li, "Ab Initio Two-Component Ehrenfest Dynamics," *J. Chem. Phys.* 2015, 143 (11), 114105.
- (7): B. Peng, P. J. Lestrangle, **J. J. Goings**, M. Caricato, X. Li, "Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-Edge X-ray Absorption Spectroscopy," *J. Chem. Theory Comput.* 2015, 11 (9), 4146–4153.
- (6): **J. J. Goings**, F. Ding, M. J. Frisch, X. Li, "Stability of the Complex Generalized Hartree-Fock Equations," *J. Chem. Phys.* 2015, 142 (15), 154109.
- (5): F. Ding, **J. J. Goings**, M. J. Frisch, X. Li, "Ab Initio Non-Relativistic Spin Dynamics," *J. Chem.*

Phys. 2014, 141 (21), 214111.

(4): J. J. Goings, A. M. Schimpf, J. W. May, R. W. Johns, D. R. Gamelin, X. Li, "Theoretical Characterization of Conduction-Band Electrons in Photodoped and Aluminum-Doped Zinc Oxide (AZO) Quantum Dots," *J. Phys. Chem. C* 2014, 118 (46), 26584–26590.

(3): J. J. Goings, M. Caricato, M. Frisch, X. Li, "Assessment of Low-Scaling Approximations to the Equation of Motion Coupled-Cluster Singles and Doubles Equations," *J. Chem. Phys.* 2014, 141 (16), 164116.

(2): J. J. Goings, S. Ohlsen, K. Blaisdell, D. Schofield, "Sorption of H₂ to Open Metal Sites in a Metal Organic Framework: A Symmetry Adapted Perturbation Analysis," *J. Phys. Chem. A* 2014, 118 (35), 7411–7417.

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

Presentations

2018: "Propensity for Proton Relay and Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor" Poster Presentation. GRC on Computational Chemistry, West Dover.

2017: "Can quantized vibrational effects be obtained from Ehrenfest mixed quantum-classical dynamics?" Oral Presentation. 253rd ACS National Meeting, San Francisco.

2016: "Real Time Propagation of the Exact Relativistic Two-Component Equations" Poster Presentation. TACC 2016, Seattle.

2016: "Recent advances in real-time TDDFT for the description of optical activity" Poster Presentation. LUEST 2016, Telluride.

2016: "Towards a Real-Time Description of Magnetic Systems with Applications to Magnetic Circular Dichroism Spectroscopy." Poster Presentation. 251st ACS National Meeting, San Diego.

2015: "Theoretical investigation of magnetic exchange interactions in dilute magnetic semiconductor quantum dots induced by defects." Oral Presentation. Pacifichem 2015, Honolulu.

2015: "Linear Response Complex Generalized Hartree-Fock." Oral Presentation. 249th ACS National Meeting, Denver.

2014: "Equation of motion formalism of second order many-body perturbation theory (EOM-MBPT2) and second-order approximate coupled-cluster (CC2)." Oral Presentation. 248th ACS National Meeting, San Francisco.

2014: "Low-Scaling Approximations to the Equation of Motion Coupled-Cluster Singles and Doubles Equations." Oral Presentation. TSRC Excited States and Time-Dependent Electronic Structure Theory, Telluride.