Joshua Goings | Curriculum Vitae

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Education

PhD Theoretical Chemistry — **University of Washington**
Advisor: Prof. Xiaosong Li — *June 2017*

BS Chemistry & Biochemistry — **Seattle Pacific University**
Summa Cum Laude — *June 2012*

Professional Experience

Postdoctoral Research Associate — **University of Illinois Urbana-Champaign**
Advisor: Prof. Sharon Hammes-Schiffer — *August 2017 – present*

Postdoctoral Research Associate — **University of Washington**
Advisor: Prof. Xiaosong Li — *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

(19): **J. J. Goings**, P. J. Lestrange, 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. Lestrange, **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 H_2 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

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.

Professional Societies

2013–: American Chemical Society (ACS), Member

Software Contributions

`Chronus Quantum`: open-source real-time time-dependent Hartree Fock module to simulate various time-resolved molecular spectroscopies.

`Gaussian`: Real-Time Electronic Dynamics (RT-TDDFT and RT-HF). Efficient (P-)EOM-MBPT2 modules for computing accurate molecular excited state properties.

Computer skills

`FORTRAN`, `python`, `C++`, LaTeX, `Linux`/Shell