

# Joshua Goings | Curriculum Vitae

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Last Updated: June 16, 2016

## Education

<b>University of Washington</b> <i>PhD Theoretical Chemistry, Advisor: Prof. Xiaosong Li</i>	<b>Seattle</b> 2012–2017
<b>Seattle Pacific University</b> <i>Dual BS Chemistry &amp; Biochemistry, GPA – 3.93/4.00, Summa Cum Laude</i>	<b>Seattle</b> 2008–2012

## Research Interests

- Development of first-principles electronic dynamics including multiple electromagnetic fields.
- Development of relativistic many body methods for magnetic and heavy-element materials.
- Electromagnetic response properties of dilute magnetic semiconductor quantum dots.
- Simulation of high-resolution spectroscopy and femtochemistry for photovoltaics and spintronics.

## 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

- (12): F. Egidi, **J. J. Goings**, M. J. Frisch, X. Li, "Relativistic Two-Component Linear Response Methods for Calculating Excited State Fine Structures," 2016, *Under Review*.
- (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. Wiegold, J. Lyding, X. Li, M. Gruebele, "Imaging Excited Orbitals of Quantum Dots: Experiment and Electronic Structure Theory", 2015, *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. Lestrage, **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<sub>2</sub> 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

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- 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. 251<sup>st</sup> ACS National Meeting, San Diego.
- 2015: "Theoretical investigation of magnetic exchange interactions in dilute magnetic semiconductor quantum dots induced by defects." Oral Presentation. Pacificchem 2015, Honolulu.
- 2015: "Linear Response Complex Generalized Hartree-Fock." Oral Presentation. 249<sup>th</sup> 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. 248<sup>th</sup> 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

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- 2013–: American Chemical Society (ACS), Member
- 2012–: Society for Industrial and Applied Mathematics (SIAM), Member

## Software Contributions

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**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

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**Advanced:** FORTRAN, python, gnuplot,  $\text{\LaTeX}$ , MATLAB, UNIX/Shell

**Basic:** C++, javascript