David Williams–Young

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OBJECTIVE

To obtain a research position relating to chemical theory and computation.

RESEARCH INTERESTS

- Development of low–scaling relativistic electronic structure methods to describe strongly correlated systems, such as transition metal complexes commonly found in the vicinity of the active sites of enzymes.
- Application of abstract mathematical paradigms, such as algebraic topology, to develop elegant and novel solutions to the problems that arise in ab initio electronic structure theory.
- Development of high–performance algorithms to treat the electronically non–adiabatic dynamics of quantum molecular systems.

EDUCATION

Doctor of Philosophy (Pursuant), Chemistry — (Projected) May 2018
University of Washington, Seattle, WA
Adviser: Dr. Xiaosong Li

Bachelor of Science (Magna Cum Laude), Chemistry, Mathematics — May 2013
Indiana University of Pennsylvania, Indiana, PA
Adviser: Dr. Jaeju Ko

PROFESSIONAL EXPERIENCE

Graduate Research Assistant — July 2013 – Present
University of Washington, Seattle, WA

Graduate Teaching Assistant — September 2013 – Present
University of Washington, Seattle, WA

- Provided supplementary lecture instruction for the undergraduate General Chemistry course series as well as full instruction for the associated lab coursework. This job entailed full responsibility for two sections of thirty students during a supplemental lecture series referred to as a quiz section. I was responsible for the evaluation of students' performance both in lecture coursework (exams, homework assignments) as well as the lab (lab reports).
- Provided supplementary lecture instruction for the final lecture course (in a series of three) of the undergraduate Organic Chemistry course series. Primarily, I was responsible for evaluating students' performance on Exams. In addition, I was responsible for making myself available for course related questions through structured office hours.
- Aided in the development of new course material for the second lecture course (in a series of two), of the graduate Quantum Chemistry course series. The developed course material focused on the practical development of basic quantum chemical methods, such as Hartree-Fock and Density Functional Theory,

using the MATLAB development environment. The students developed, from scratch, a working implementation of these methods with the aid of provided course material developed by my self and the primary course instructor. For this course, I also had the primary responsibility for evaluating students' progress through the grading of exams and assigned course work.

Undergraduate Research Assistant September 2011 – May 2013
Indiana University of Pennsylvania, Indiana, PA

Chemistry Tutor August 2010 – May 2011
Indiana University of Pennsylvania Disability Services, Indiana, PA

- Provided supplemental course instruction for the General and Organic Chemistry series for students with disabilities. This primarily entailed meeting with students individually on a weekly basis to aid in their understanding of course material and to ensure that they were not falling behind in coursework.

Information Technology Technician August 2009 – January 2010
Central Michigan University Information Technology, Mt. Pleasant, MI

- Primarily responsible for solving network connectivity issues for incoming students at Central Michigan University.

COMPUTATIONAL PROFICIENCY

I am very proficient in the following computational areas:

- *Programming Languages:* C/C++/C#, FORTRAN 77/95/03, Java
- *Scripting Languages:* Python, Julia, R, MATLAB, Octave, C/Bash Shell
- *Libraries / Paradigms:* OpenMP, TBB, MPI, OpenGL, CUDA, OpenACC, PThreads
- *Software:* Gaussian, Mathematica, MATLAB

I have contributed to the development of the following software packages:

- Chronus Quantum Chemistry (ChronusQ) Software Package (*Principle Developer*)
- Gaussian (*Contributor*)
  - Analytical hessians of time–dependent density functional theory
  - Chebyshev expansion of the quantum propagator in real–time density functional theory

PUBLICATIONS

4 in press publications, 2 as first author

* Indicates equal contribution to published work

10. **Williams–Young, D. B.**; Scalmani, G.; Sun, S.; Frisch, M.; Li, X.; "*On the Accurate and Efficient Evaluation of the Analytical Hessians of Electronically Excited States within the Random Phase Approximation*" **2017**, In Preparation.
9. **Williams–Young, D. B.**; Hongbin Liu; Li, X.; "*Time–Dependent Density Functional Theory (TD-DFT) Benchmark of Excited–State Polarizabilities*" **2017**, In Preparation.
8. Van Beeuman, R.; **Williams–Young, D. B.**; Kasper, J.; Yang, C.; Ng, E. G.; Li, X.; "*A Model Order Reduction Algorithm for Estimating the Absorption Spectrum*" **2017**, Submitted..
7. Egidi, F.*; **Williams–Young, D. B.***; Baiardi, A.*; Bloino, J.; Scalmani, G.; Frisch, M.; Li, X.; Barone, V.; "*Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: the VPT2-TDDFT Route*" *J. Chem. Theor. Comp.*, **2017**, Submitted.
6. Petrone, A.*; **Williams–Young, D. B.***; Lingerfelt, D. B.; Li, X.; "*Ab Initio Transient Raman Analysis*" *J. Phys. Chem. A.*, **2017**, Submitted.

5. **Williams–Young, D. B.***; Lingerfelt, D. B.*; Petrone, A.; Li, X.; "*Ab Initio Surface Hopping Dynamics within the Particle-Particle Tamm–Dancoff Approximation*" *J. Chem. Phys. Comm.*, **2017**, *Submitted.*

4. Petrone, A.; Lingerfelt, D. B.; **Williams–Young, D. B.**; Li, X.; "*Ab Initio Transient Vibrational Spectral Analysis*" *J. Phys. Chem. Lett.*, **2016**, 7, 4501–4508.

3. **Williams–Young, D. B.**; Goings, J.; Li, X.; "*Accelerating Real–Time Time-Dependent Density Functional Theory with a Non–Recursive Chebyshev Expansion of the Quantum Propagator*" *J. Chem. Theor. Comp.*, **2016**, 12(11) 5333–5338.

2. **Williams–Young, D. B.**; Egidi, F.; Li, X.; "*Relativistic Two-Component Particle-Particle Tamm–Dancoff Approximation*" *J. Chem. Theor. Comp.*, **2016**, 12(11), 5379–5384.

1. Lingerfelt, D. B.; **Williams–Young, D. B.**; Petrone, A; Li, X.; "*Direct ab Initio (Meta-)Surface-Hopping Dynamics*", *J. Chem. Theor. Comp.*, **2016**, 12(3), 935–945.

CURRENT SOFTWARE CITATIONS

3. Li, X.; Valeev, E. F.; **Williams–Young, D. B.**; Ding, F.; Liu, H.; Goings, J. J.; Petrone, A.; Lestrange, P.; *Chronus Quantum, Beta Version*, `http://www.chronusquantum.org`, **2016**.

2. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Izmaylov, A. F.; Sonnenberg, J. L.; **Williams–Young, D. B.**; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Ortiz, J. V.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; and Fox , D. J.; *Gaussian Development Version, Revision I.09*, Gaussian, Inc., Wallingford CT, **2016**.

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Izmaylov, A. F.; Sonnenberg, J. L.; **Williams–Young, D. B.**; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Ortiz, J. V.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; and Fox , D. J.; *Gaussian 16, A.03*, Gaussian, Inc., Wallingford CT, **2016**.

HONORS

MolSSI Software Fellow — Molecular Sciences Software Institute (2017)
Nicole A. Boand Endowed Fellowship in Chemistry — ARCS Foundation (2016)
Early Bird Research Assistantship (EBRA) — University of Washington (2013)
Excellence in Chemistry Graduate Fellowship Award (ECGFA) — University of Washington (2013)
Provost Scholar — Indiana University of Pennsylvania (2013)

PRESENTATIONS

* Indicates an invited presentation

∗9. **Williams–Young, D. B.**; "*Studying Semi–Classical Molecular Light–Matter Interaction through Time–Dependent Density Function Theory*"; High Performance Computing Seminar, University of Washington. **2017**. Oral Presentation.

8. **Williams–Young, D. B.**; Goings, J. J.; Li, X.; "*Accelerating Real–Time Time–Dependent Density Functional Theory with a Chebyshev Expansion of the Quantum Propagator*"; Theory and Applications of Computational Chemistry (TACC) 2016, Seattle, WA. **2016**. Poster.

7. Egidi F.; **Williams–Young, D. B.**; Li, X.; "*Electronic Structure Methods for Relativistic Effects in Excited States*"; Low Scaling and Unconventional Electronic Structure Theory (LUEST) 2016, Telluride, CO. **2016**. Poster.

6. **Williams–Young, D. B.**; Yang, W.; Li, X.; "*Moving past the particle-hole description of excited states: Affordable methodologies*"; Chemical Congress of Pacific Basin Societies (PacifiChem) 2015, Honolulu, HI. **2015**. PHYS: Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics. Oral Presentation.

5. **Williams–Young, D. B.**; Ko, J.; Ondrechen, M. J.; "*Computational approach to the prediction of enzyme specificities*"; 245th American Chemical Society National Meeting & Exposition, New Orleans, LA. **2013**. Sci-Mix Poster Session. Poster.

4. **Williams–Young, D. B.**; Ko, J.; Ondrechen, M. J.; "*Computational approach to the prediction of enzyme specificities*"; 245th American Chemical Society National Meeting & Exposition, New Orleans, LA. **2013**. Division of Computers in Chemistry Poster Session. Poster.

3. **Williams–Young, D. B.**; Ko, J.; "*Prediction of Relative Activities of Enzymes using Computed Chemical Properties*"; American Chemical Society Student Member Symposium, Duquesne University. Duquesne, PA. **2012**. Poster.

2. **Williams–Young, D. B.**; Ko, J.; "*Prediction of Relative Activities of Enzymes using Computed Chemical Properties*"; Undergraduate Research Forum, Indiana University of Pennsylvania. Indiana, PA. **2012**. Poster.

1. Ford, J.; Ko, J.; Mintmier, B.; Machovia, T.; Kang, M.; Owens, A.; **Williams–Young, D. B.**; "*Undergraduate Research in Biomass Utilization Symposium*", Pennsylvania Association of the Council of Trustees Conference, Indiana University of Pennsylvania. Indiana, PA. **2011**. Oral Presentation.

MEMBERSHIPS

Alpha Chi Sigma (AXΣ), ΓT Chapter, Professional Chemistry Fraternity
American Chemical Society (ACS), Computers in Chemistry Division

INTERESTS

World percussion, kayaking, hiking, climbing, Linux kernel development