David Williams–Young

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Computational Research Division
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OBJECTIVE

To obtain a research position relating to high–performance scientific computing and numerical linear algebra.

RESEARCH INTERESTS

- Development of high–performance and reduced scaling relativistic electronic structure methods.
- Algorithmic development for high–performance quaternionic linear algebra software.
- 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.

EDUCATION

Doctor of Philosophy, Chemistry — May 2018
University of Washington, Seattle, WA
Adviser: Dr. Xiaosong Li
Thesis: *Towards Efficient and Scalable Electronic Structure Methods for the Treatment of Relativistic Effects and Molecular Response*

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

PROFESSIONAL EXPERIENCE

Postdoctoral Fellow — July 2018 – Present
Scalable Solvers Group
Department of Applied Mathematics
Computational Research Division
Lawrence Berkeley National Laboratory
Berkely, CA

Graduate Research Assistant — July 2013 – July 2018
University of Washington, Seattle, WA

Graduate Teaching Assistant — September 2013 – July 2018
University of Washington, Seattle, WA

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

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

COMPUTATIONAL PROFICIENCY

I am very proficient in the following computational areas:

- *Programming Languages:* C++, C, FORTRAN 77/95/03, Java, C#
- *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

12 in press publications, 2 as first author, 3 as equally contributing author

* Indicates equal contribution to published work

12. Sun, S.; **Williams–Young, D. B.**; Stetine, T.F.; Li, X.; "*Generalized Hartree-Fock with a Non-perturbative Treatment of Strong Magnetic Fields: Application to Molecular Spin Phase Transitions*"; *J. Chem. Theor. Comp.*, **2018**, Just Accepted.
11. Petrone, A.*; **Williams–Young, D. B.***; Sun, S.; Stetina, T. F.; Li, X.; "*An Efficient Implementation of Two-Component Relativistic Density Functional Theory with Torque-Free Auxiliary Variables*"; *Eur. Phys. J. B*, **2018**, 91(7), 169.
10. Kasper, J.; **Williams–Young, D. B.**; Vecharynski, E.; Yang, C.; Li, X.; "*A Well-Tempered Hybrid Method for Solving Challenging TDDFT Systems*"; *J. Chem. Theor. Comp.*, **2018**, 14(4), 2034–2041.
9. Lestrange, P.; **Williams–Young, D. B.**; Jimenez–Hoyos, C.; Li, X.; "*An Efficient Implementaion of Variation After Projection Generalized Hartree–Fock*" *J. Chem. Theor. Comp.*, **2018**, 14(2), 588–596.
8. Barclay, M. S.; Quincy, T. J.; **Williams–Young, D. B.**; Caricato, M.; Elles, C. G.; " *Accurate Assignments of Excited-State Resonance Raman Spectra: A Benchmark Study Combining Experiment and Theory*" *J. Phys. Chem. A.*, **2017**, 121(41), 7937–7946.
7. 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*" *J. Chem. Theor. Comp.*, **2017**, 13(10), 4950–4961.
6. 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**, 13(6), 2789–2803.
5. Petrone, A.*; **Williams–Young, D. B.***; Lingerfelt, D. B.; Li, X.; "*Ab Initio Transient Raman Analysis*" *J. Phys. Chem. A.*, **2017**, 121(20), 3958–3965.
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. **Williams–Young, D. B.**; *HAXX: Hamilton's Quaternion Algebra for CXX*, `http://github.com/wavefunction91/HAXX`, **2017**.
2. 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**.
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

CCG Excellence Award for Graduate Students	The Chemical Computing Group (2017)
MolSSI Software Fellow	Molecular Sciences Software Institute (2017-2018)
Lloyd E. and Florence M. West Fellowship in Chemistry	Lloyd E. and Florence M. West (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

10. **Williams–Young, D. B.**; van Beeuman, R.; Yang, C.; Li, X.; "*A Novel Model Reduction Algorithm for the Efficient Evaluation of Molecular Response Properties*"; 254th American Chemical Society National Meeting & Exposition, Washington, D.C. **2017**. Poster.
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 (ΑΧΣ), ΓΤ Chapter, Professional Chemistry Fraternity
American Chemical Society (ACS), Computers in Chemistry Division

INTERESTS

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