David Williams–Young

Academic Address
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 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 (Ph.D.), Chemistry — May 2018
University of Washington, Seattle, WA
Adviser: Dr. Xiaosong Li
Dissertation: *Towards Efficient and Scalable Electronic Structure Methods for the Treatment of Relativistic Effects and Molecular Response*

Bachelor of Science (B.S., *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

COMPUTATIONAL PROFICIENCY

I am a specialist in the following computational areas:

- *Programming Languages:* C++, C, FORTRAN 77/95/03
- *Libraries / Paradigms:* OpenMP, MPI, PThreads
- *Software:* Gaussian

I am very proficient in the following computational areas:

- *Programming Languages:* Java, C#
- *Scripting Languages:* Python, Julia, R, MATLAB, Octave, C/Bash Shell
- *Libraries / Paradigms:* TBB, OpenGL, CUDA, OpenACC
- *Software:* Mathematica, MATLAB

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

- The Chronus Quantum (ChronusQ) Software Package (*Principle Developer*)
- NWChemEx (*Contributor*)
- Gaussian (*Contributor*)

PUBLICATIONS

19 in press publications, 3 as first author, 3 as equally contributing (first) author, 1 invited.

* Indicates equal contribution to published work.

† Indicates that the publication was invited.

19. Koulias, L.N.; **Williams–Young, D. B.**; Nascimento, D.R.; DePrince, A.E.; Li, X.; "*Relativistic Real-Time Time-Dependent Equation-of-Motion Coupled-Cluster*" *J. Chem. Theor. Comp.*, **2019**, 15(12), 6617–6624.
18. Sun, S.; Beck, R.; **Williams–Young, D. B.**; Li, X.; "*Simulating Magnetic Circular Dichroism Spectra with Real-Time Time-Dependent Density Functional Theory in Gauge Including Atomic Orbitals*" *J. Chem. Theor. Comp.*, **2019**, 15(12), 6824–6831.
17. † **Williams–Young, D. B.**; Petrone, A.; Sun, S.; Stetina, T.F.; Lestrange, P.; Hoyer, C.E.; Nascimento, D.R.; Koulias, L.; Wildman, A.; Kasper, J.; Goings, J.J.; Ding, F.; DePrince, A.E.; Valeev, E.F.; Li, X.; "*The Chronus Quantum (ChronusQ) Software Package*" *WIREs Comput. Mol. Sci.* **2019**, e1436.
16. Stetina, T.F.; Sun, S.; **Williams–Young, D. B.**; Li, X.; "*Modeling Magneto-Photoabsorption Using Time-Dependent Complex Generalized Hartree-Fock*" *ChemPhotoChem*, **2019**, 3(9), 739–746.
15. Hoyer, C.; **Williams–Young, D. B.**; Huang, C.; Li, X.; "*Embedding Non-Collinear Two-Component Electronic Structure in a Collinear Quantum Environment*" *J. Chem. Phys.*, **2019**, 150(17), 174114.
14. Peng, B.; Van Beeumen, R.; **Williams–Young, D. B.**; Kowalski, K.; Yang, C.; "*Approximate Green's Function Coupled Cluster Method Employing Effective Dimension Reduction*"; *J. Chem. Theor. Comp.*, **2019**, 15(5), 3185–3196.
13. Sun, S.; **Williams–Young, D. B.**; Li, X.; "*An Ab Initio Linear Response Method for Computing Magnetic Circular Dichroism Spectra with Non-Perturbative Treatment of Magnetic Field*"; *J. Chem. Theor. Comp.*, **2019**, 15(5), 3162–3169.
12. Sun, S.; **Williams–Young, D. B.**; Stetina, 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.*, **2019**, 15(1), 348–356.
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`, **2019**.
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`, **2019**.
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)

PROFESSIONAL SERVICE

Reviewer, *The Journal of Chemical Theory and Computation*	(2019)
Reviewer, *Journal of Computational Physics*	(2019)

PRESENTATIONS

* Indicates an invited presentation

12. **Williams–Young, D. B.**; Van Beeuman, R.; Yang, C.; Li, X.; "*A General Model Order Reduction Scheme for the Evaluation of Spectroscopic Properties and Excited States*"; American Physical Society March Meeting 2019, Boston, MA. **2019**. Oral Presentation.
11. * **Williams–Young, D. B.**; "*On the High Performance Implementation of Quaternionic Matrix Operations*"; Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering (SIAM-CSE19), Spokane, WA. **2019**. Oral 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 (AXΣ), ΓT Chapter, Professional Chemistry Fraternity
American Chemical Society (ACS), Computers in Chemistry Division
American Physical Society (APS)
Society for Industrial and Applied Mathematics (SIAM), Computer Science and Engineering Division

INTERESTS

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