

David Williams–Young

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OBJECTIVE

To obtain a research position relating to high–performance scientific computing and numerical linear algebra and their interplay with methods development in electronic structure theory.

RESEARCH INTERESTS

- Development of high–performance and reduced scaling electronic structure methods on emerging architectures (GPUs, FPGAs, etc).
- Algorithmic development for high–performance linear algebra software (Krylov solvers).
- Application of abstract mathematical paradigms, such as algebraic topology and differential geometry, 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, Berkeley, 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

COMPUTATIONAL PROFICIENCY

I am a specialist in the following computational areas:

- *Programming Languages*: C++
- *Libraries / Paradigms*: OpenMP, MPI, BLAS/LAPACK, CUDA

I am very proficient in the following computational areas:

- *Programming Languages*: C, FORTRAN 77/95/03
- *Scripting Languages*: Python, Julia, Octave, C/Bash Shell
- *Libraries / Paradigms*: TBB, 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

21 in press publications, 1 accepted pending publication, 2 submitted manuscripts, 6 as first author (named), 3 as equally contributing (first) author, 2 invited.

* Indicates equal contribution to published work.

† Indicates that the publication was invited.

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2018-Present

6. Kowalski, K.; Aprà, E.; Bair, R.; Boschen, J.; Bylaska, E.; Daily, J.; de Jong, W.; Dunning, T.; Govind, N.; Harrison, R.; Keipert, K.; Krishnamoorthy, S.; Kumar, S.; Mutlu, E.; Palmer, B.; Panyala, A.; Peng, B.; Richard, R.; Straatsma, T.; Valeev, E.; Valiev, M.; van Dam, H.; **Williams–Young, D. B.**; Yang, C.; Zalewski, M.; Windus, T.; “*NWChemEx—Computational Chemistry for the Exascale Era*”; *Chemical Reviews*, **2020**, Submitted.
5. Ahmed, H.; **Williams–Young, D. B.**; Ibrahim, K.Z.; Yang, C.; “*Performance Modeling and Tuning for DFT Calculations on Heterogeneous Architectures*”; *International Symposium on Computer Architecture and High Performance Computing*, **2020**, Submitted.
4. † **Williams–Young, D. B.**; de Jong, W.A.; van Dam, H.J.J.; Yang, C.; “*On the Efficient Evaluation of the Exchange Correlation Potential on Graphics Processing Unit Clusters*”; *Frontiers in Chemistry*, **2020**, Accepted.
3. **Williams–Young, D. B.**; Beckman, P.G.; Yang, C.; “*A Shift Selection Strategy for Parallel Shift-Invert Spectrum Slicing in Symmetric Self-Consistent Eigenvalue Computation*”; *ACM Trans. Math. Soft.*, **2020**, 46, 4, Article 35 (September 2020).
2. **Williams–Young, D. B.**; Yang, C.; “*Parallel Shift-Invert Spectrum Slicing on Distributed Architectures with GPU Accelerators*” in *Proceedings of the 49th International Conference on Parallel Processing (ICPP’20)*, **2020**.
1. 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.

18. 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.
17. 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.
16. † **Williams–Young, D. B.**; Petrone, A.; Sun, S.; Stetina, T.F.; Lestrangle, 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.
15. 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.
14. 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.
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. Lestrangle, P.; **Williams–Young, D. B.**; Jimenez-Hoyos, C.; Li, X.; “*An Efficient Implementation 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.

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, <i>The Journal of Chemical Theory and Computation</i>	(2019)
Reviewer, <i>Journal of Computational Physics</i>	(2019)
Reviewer, <i>The Journal of Chemical Physics</i>	(2020)
Reviewer, <i>The International Journal of Quantum Chemistry</i>	(2020)
Reviewer, <i>Computer Physics Communications</i>	(2020)
Minisymposium Organizer, <i>SIAM Conference on Parallel Processing for Scientific Computing</i>	(2020)

PRESENTATIONS

* Indicates an invited presentation

11. **Williams–Young, D. B.**; Yang, C.; “*Parallel Shift-Invert Spectrum Slicing for Symmetric Self-Consistent Eigenvalue Computation*”; Society for Industrial and Applied Mathematics Conference on Parallel Processing for Scientific Computing (SIAM-PP20), Seattle, WA. **2020**. Oral Presentation.
10. **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.
9. * **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. **2019**. Oral Presentation
8. **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.
7. * **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.
6. **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.
5. **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.

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**. Sci-Mix Poster Session. Poster.
3. **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.
2. **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.
1. **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.

MEMBERSHIPS

Alpha Chi Sigma (AXΣ), IT 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