David Williams–Young

Research Scientist (Career),
Applied Commputing for Scientific Discovery Group (ACSD),
Applied Mathematics and Computational Research Division (AMCR),
Lawrence Berkeley National Laboratory
50F-1645 (office), MS 50F-1650 (mail)
1 Cyclotron Road, Berkeley, CA 94720
+1 (510) 495-2189
dbwy@lbl.gov

RESEARCH INTERESTS

- Development of high–performance and reduced scaling electronic structure methods on emerging architectures (GPUs, FPGAs, etc).
- Development of novel field-theoretic methods for the elucidation of relativistic electronic structure in superheavy elements.
- Development of novel quantum algorithms for the simulation of the relativistic many-body problem.
- The intersection of high-performance computing and quantum information science.
- Algorithmic development for high–performance, sparse linear algebra software (Krylov solvers).

PROFESSIONAL EXPERIENCE

Research Scientist (Career) ..... March 2023 – Present
Research Scientist (Career-Track) ..... February 2021 – March 2023
Postdoctoral Fellow ..... July 2018 – February 2021
Applied Mathematics and Computational Research Division
Lawrence Berkeley National Laboratory, Berkeley, CA

Graduate Research Assistant ..... July 2013 – July 2018
Graduate Teaching Assistant ..... September 2013 – July 2018
Department of Chemistry
University of Washington, Seattle, WA

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

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

COMPUTATIONAL PROFICIENCY

I am a specialist in the following computational areas:

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

I am very proficient in the following computational areas:

- *Programming Languages:* C, FORTRAN 77/95/03, HIP, SYCL
- *Scripting Languages:* Python, Julia, Octave, C/Bash Shell
- *Libraries / Paradigms:* TBB, OpenACC
- *Software:* Mathematica, MATLAB

I am the primary developer of the following open-source software packages:

- **GauXC**: Enabling high-performance density functional theory calculations on exascale architectures
- **MACIS**: Massively parallel selected configuration interaction methods
- **ExchCXX**: GPU-accelerated library for the evaluation of exchange-correlation functionals

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

- The Chronus Quantum (ChronusQ) Software Package
- NWChemEx
- Massively Parallel Quantum Chemistry (MPQC4)
- TiledArray
- Gaussian

PUBLICATIONS

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

* Indicates equal contribution to published work.

† Indicates that the publication was invited.

Lawrence Berkeley National Laboratory 2018-Present

23. Hirsbrunner, M.R.; Mullinax, J.W.; Shen, Y.; **Williams–Young, D. B.**; Klymko, K.; Van Beeumen, R.; Tubman, N.M.; "*Diagnosing local minima and accelerating convergence of variational quantum eigensolvers with quantum subspace techniques*" **2024**. Submitted.
22. Alvertis, A.M.; **Williams–Young, D. B.**; Bruneval, F; Neaton, J.B.; "*Capturing electronic correlations in electron-phonon interactions in molecular systems with the GW approximation*" **2024**. Submitted.
21. Shen, Y.; Camps, D.; Szaz, A.; Darbha, S.; Klymko, K.; **Williams–Young, D. B.**; Tubman, N.B.; Van Beeumen, R.; "*Estimating Eigenenergies from Quantum Dynamics: A Unified Noise-Resilient Measurement-Driven Approach*" **2023**. Submitted.
20. † Blum, V.; Asahi, R.; Autschbach, J.; Bannwarth, C.; Bihlmayer, G.; Blügel, S.; Burns, L. A.; Crawford, T. D.; Dawson, W.; de Jong, W. A.; Draxl, C.; Filippi, C.; Genovese, L.; Giannozzi, P.; Govind, N.; Hammes-Schiffer, S.; Hammond, J. R.; Hourahine, B.; Jain, A.; Kanai, Y.; Kent, P. R. C.; Larsen, A. H.; Lehtola, S.; Li, X.; Lindh, R.; Maeda, S.; Makri, N.; Moussa, J.; Nakajima, T.; Nash, J. A.; Oliveira, M. J. T.; Patel, P. D.; Pizzi, G.; Pourtois, G.; Pritchard, B. P.; Rabani, E.; Reiher, M.; Reining, L.; Ren, X.; Rossi, M.; Schlegel, H. B.; Seriani, N.; Slipchenko, L. V.; Thom, A.; Valeev, E. F.; Van Troeye, B.; Visscher, L.; Vlcek, V.; Werner, H.-J.; **Williams–Young, D. B.**; Windus, T. "*Roadmap on methods and software for electronic structure based simulations in chemistry and materials*" *Electronic Structure*; **2024**. Accepted.

19. **Williams–Young, D. B.**; Yuwono, S.; DePrince III, A.E.; Yang, C.; "*Approximate Exponential Integrators for Time-Dependent Equation-of-Motion Coupled Cluster Theory*" *J. Chem. Theory Comput.*; **2023**. 19, 24, 9177–9186.

18. Di Felice, R.; Mayes, M.; Richard, R.; **Williams–Young, D. B.**; Chan, G.K.L; de Jong, W.A.; Govind, N.; Head-Gordon, M.; Hermes, M.; Kowalski, K.; Li, X.; Lischka, H.; Mueller, K.; Mutlu, E.; Niklasson, A.; Pederson, M.; Peng, B.; Shepard, R.; Valeev, E.; van Schilfgaarde, M.; Vlaisavljevich, B.; Windus, T.; Xantheas, S.; Zhang, X.; Zimmerman, P.; "*A Perspective on Sustainable Computational Chemistry Software Development and Integration*" *J. Chem. Theory Comput.*; **2023**. 19, 20, 7056–7076.

17. Ko, T.; Heindel, J.; Guan, X.; Head-Gordon, T.; **Williams–Young, D. B.**; Yang, C.; "*Using Diffusion Maps to Analyze Reaction Dynamics for a Hydrogen Combustion Benchmark Dataset*" *J. Chem. Theory Comput.*; **2023**. 19, 17, 5872–5885.

16. † **Williams–Young, D. B.**; Asadchev, A.; Popovici, D.T; Clark, D.; Waldrop, J.; Windus, T.L.; Valeev, E.F.; de Jong, W.A.; "*Distributed Memory, GPU Accelerated Fock Construction for Hybrid, Gaussian Basis Density Functional Theory*"; *J. Chem. Phys.*; **2023**. 158, 234104.

15. † **Williams–Young, D. B.**; Tubman, N.M.; Mejuto-Zaera, C.; de Jong, W.A.; "*A Parallel, Distributed Memory Implementation of the Adaptive Sampling Configuration Interaction Method*"; *J. Chem. Phys.*; **2023**. 158, 214109.

14. Richard, R.; Keipert, K.; Waldrop, J.; Keçeli, M.; **Williams–Young, D. B.**; Bair, R.; Boschen, J.; Crandall, Z.; Gasperich, K.; Mahmud, Q.; Panyala, A.; Valeev, E.F.; van Dam, H,; de Jong, W.A.; Windus, T.; "*PluginPlay: Enabling Exascale Scientific Software One Module at a Time*"; *J. Chem. Phys.*; **2023**. 158, 184801.

13. Shen, Y.; Klymko, K.; Sud, J.; **Williams–Young, D. B.**; de Jong, W.A.; Tubman, N.M; "*Real-Time Krylov Theory for Quantum Computing Algorithms*"; **2023**. *Quantum.* 7, 1066.

12. Gomes, N.; **Williams–Young, D. B.**; de Jong, W.A.; "*Computing the Many-Body Green's Function with Adaptive Variational Quantum Dynamics*"; *J. Chem. Theory Comput.*; **2023**. 19, 11, 3313–3323.

11. Sid-Lakhdar, W.M.; Cayrols, S.; Bielich, D.; Abdelfattah, A.; Luszczek, P. Gates, M.; Tomov, S.; Johansen, H.; **Williams–Young, D. B.**; Davis, T.; Dongerra, J.; Anzt, H.; "*PAQR: Pivoting Avoiding QR factorization*"; 2023 IEEE International Parallel and Distributed Processing Symposium (IPDPS), St. Petersburg, FL, USA; **2023**, pp. 322-332.

10. Mejuto-Zaera, C.; Tzeli, D; **Williams–Young, D. B.**; Tubman, N.M.; Matoušek, M.; Brabec, J.; Veis, L.; Xantheas, S; de Jong, W.A.; "*The Effect of Geometry, Spin and Orbital Optimization in Achieving Accurate, Fully-Correlated Results for Iron-Sulfur Cubanes*"; *J. Chem. Theory Comput*; **2022**. 18(2), 687–702.

9. Bez, J.L.; Tang, H.; Xie, B.; **Williams–Young, D. B.**; Latham, R.; Ross, R.; Oral, S.; Byna, S.; "*I/O Bottleneck Detection and Tuning:Connecting the Dots using Interactive Log Analysis*"; *2021 IEEE/ACM 6th International Parallel Data Systems Workshop (PDSW)*, **2021**.

8. **Williams–Young, D. B.**; Bagusetty, A.; de Jong, W.A.; Doerfler, D.; vam Dam, H.J.J.; Vazquez–Mayagoitia, A.; Windus, T.L.; Yang, C.; "*Achieving Performance Portability in Gaussian Basis Set Density Functional Theory on Accelerator Based Architectures*"; *Parallel Computing*, **2021**, 108, 102829.

7. Ahmed, H.; **Williams–Young, D. B.**; Ibrahim, K.Z.; Yang, C.; "*Performance Modeling and Tuning for DFT Calculations on Heterogeneous Architectures*"; *22nd IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC 2021)*, **2021**, pp. 714–722.

6. Kowalski, K.; Bair, R.; Bauman, N.P.; Boschen, J.S.; Bylaska, E.J.; Daily, J.; de Jong, W.A.; Dunning, T.; Govind, N.; Harrison, R.J.; Keceli, M.; Keipert, K.; Krishnamoorthy, S.; Kumar, S.; Mutlu, E.; Palmer, B.; Panyala, A.; Peng, B.; Richard, R.M.; Straatsma, T.P.; Sushko, P.; Valeev, E.F.; Valiev, M.; van Dam, H.J.J.; Waldrop, J.M.; **Williams–Young, D. B.**; Yang, C.; Zalewski, M.; Windus, T.L.; "*From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape*"; *Chemical Reviews*, **2021**, 121(8), 4962–4998.

5. Yang, C.; Brabec, J.; Veis, L.; **Williams–Young, D. B.**; Kowalski, K.; "*Solving Coupled Cluster Equations by the Newton Krylov Method*"; *Frontiers in Chemistry*, **2020**, 8:590184.
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**, 8:581058.
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.

University of Washington 2013-2018

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.; 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.
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. Lestrange, 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

Journal Review

Molecular Physics, *The Journal of Chemical Physics*, *The International Journal of Quantum Chemistry*, *Computer Physics Communications*, *The Journal of Chemical Theory and Computation*, *Journal of Computational Physics*, *The Journal of Physical Chemistry*, *The Journal of Physical Chemistry A*

Proposal Review

NSF Office of Advanced Cyberinfrastructure	(2022, 2023)
DOE Office of Science, Office of Basic Energy Sciences	(2023)
Natural Sciences and Engineering Research Council of Canada	(2023)

Conference Symposium Organization

SIAM Conference on Computational Science and Engineering	(2019, 2021, 2023)
SIAM Conference on Parallel Processing for Scientific Computing	(2020)

PRESENTATIONS

* Indicates an invited presentation

18. **Williams–Young, D. B.**; "*Revisiting Pseudospectral Methods for Hybrid Kohn-Sham Density Functional Theory in the Age of Exascale Computing*"; American Phyiscal Society March Meeting 2023; Las Vegas, NV; **2023**; Oral Presentation.
17. * **Williams–Young, D. B.**; "*Perspective on High-Performance Algorithms for Eigenvalue Problems in Physical Simulations*"; Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering (SIAM-CSE23); Amsterdam, The Netherlands; **2023**; Oral Presentation.
16. * **Williams–Young, D. B.**; "*Modular Design Patterns for the Sustainable Development of High-Performance Computational Chemistry Software*"; Basic Energy Sciences Workshop on Sustainable Computational Chemistry Software Development, Integration, and Application; Seattle, WA; **2022**; Oral Presentation.
15. * **Williams–Young, D. B.**; "*Low-Order, Scalable Eigensolvers for Electronic Structure Simulations Based on Spectrum Slicing*"; CECAM Workshop on Challenges and Advances in Solving Eigenproblems for Electronic Structure Theory; Lausanne, Switzerland; **2022**; Oral Presentation.
14. **Williams–Young, D. B.**; "*Revisiting Pseudospectral Methods for Hybrid Kohn-Sham Density Functional Theory in the Age of Exascale Computing*"; 263rd American Chemical Society National Meeting & Exposition; San Diego, CA; **2022**; Oral Presentation.
13. **Williams–Young, D. B.**; "*Developing (Semi)numerical Methods for Hybrid Kohn-Sham Density Functional Theory in the Age of Exascale Computing*"; The International Chemical Congress of Pacific Basin Societies (Pacifichem '21); Virtual; **2021**; Oral Presentation.
12. * **Williams–Young, D. B.**; "*Parallel Shift-Invert Spectrum Slicing for Symmetric Self-Consistent Eigenvalue Computation*"; Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering (SIAM-CSE21); Virtual; **2021**; Oral Presentation.
11. **Williams–Young, D. B.**; "*Parallel Shift-Invert Spectrum Slicing on Computing Clusters with GPU Accelerators*"; 49th International Conference on Parallel Processing (ICPP20); Virtual; **2020**; Oral Presentation.
10. **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.
9. **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.
8. * **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.
7. **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, DC; **2017**; Poster.
6. * **Williams–Young, D. B.**; "*Studying Semi–Classical Molecular Light–Matter Interaction through Time–Dependent Density Function Theory*"; High Performance Computing Seminar; University of Washington, Seattle, WA; **2017**; Oral Presentation.
5. **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.

4. **Williams–Young, D. B.**; Yang, W.; Li, X.; "*Moving past the particle-hole description of excited states: Affordable methodologies*"; The International Chemical Congress of Pacific Basin Societies (Pacifichem '15); Honolulu, HI; **2015**; Oral Presentation.
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**; 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 (ΑΧΣ), ΓΤ Chapter, Professional Chemistry Fraternity
American Chemical Society (ACS), Computers in Chemistry Division
American Physical Society (APS)
Society for Industrial and Applied Mathematics (SIAM), Activity Group on Computational Science and Engineering