Ryan M. Richard — Chemistry

Ames National Labratory and Iowa State University – Ames, IA – USA
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https://rmrresearch.github.io/

Staff Scientist at Ames National Laboratory and Adjunct Assistant Professor of Chemistry at Iowa State University. Research interests include: *ab initio* methods development, computational chemistry, high-performance computing, high-accuracy quantum chemistry, and scientific software design.

Education

- **Ph.D. The Ohio State University** — **Columbus, OH**
  Dissertation topic: — *2008–2013*
  "Increasing the Computational Efficiency of Ab Initio Methods with Generalized Many-Body Expansions"
  Advisor: John M. Herbert
- **B.S. Cleveland State University** — **Cleveland, OH**
  Undergraduate: Chemistry major, Advisor: David W. Ball — *2004–2008*

Professional Experience

- **Scientist II, Ames National Laboratory** — **Ames, IA**
  Architect and lead developer of NWChemEx. — *2018–Present*
  Additional Responsibilities: Mentor undergraduate researchers.
- **Research Assistant, NASA Glenn Research Center** — **Cleveland, OH**
  Research Topics: — *2007–2008*
  Characterization of degradation properties of ionic liquid based lubricants for terrestrial and space applications by Raman and infrared spectroscopies as well as liquid and gas chromatography.

Academic Experience

- **Adjunct Assistant Professor of Chemistry, Iowa State University** — **Ames, IA**
  High-accuracy benchmark development. — *2022–Present*
  Additional Responsibilities: Co-advise graduate students, serve on thesis committees.
- **Postdoctoral Researcher, Ames National Laboratory** — **Ames, IA**
  Algorithm development, development of massively parallel architecture — *2017–2018*
  Additional Responsibilities: Mentor undergraduate researchers
- **Postdoctoral Researcher, Georgia Institute of Technology** — **Atlanta, GA**
  Algorithm development, high-accuracy bench marking — *2014–2017*
  Additional Responsibilities: Mentor undergraduate researchers, substitute teach lectures, assist in grant writing
- **Research Assistant, The Ohio State University** — **Columbus, OH**
  Algorithm development, excited state modeling — *2008–2014*
- **Teaching Assistant, The Ohio State University** — **Columbus, OH**
  General chemistry laboratory and recitation, physical chemistry recitation — *2009–2011*
  Additional Responsibilities: Grading, weekly office hours
- **Research Assistant, Cleveland State University** — **Cleveland, OH**
  Characterization of new high-energy materials — *2006–2008*

Software Development Experience

- **NWChemEx** https://github.com/NWChemEx-Project
  Architect and lead developer *2017–present*
  - Package focused on high-performance, massively parallel electronic structure theory.
  - Software products:
    - CHEMIST — https://github.com/NWChemEx/Chemist
    - INTEGRALS – https://github.com/NWChemEx/Integrals
    - PARALLELZONE — https://github.com/NWChemEx/ParallelZone
    - PLUGINPLAY — https://github.com/NWChemEx/PluginPlay
    - SCF – https://github.com/NWChemEx/SCF
    - SIMDE — https://github.com/NWChemEx/SimDE
    - TENSORWRAPPER — https://github.com/NWChemEx/TensorWrapper
- **GhostFragment** https://github.com/rmrresearch/GhostFragment
  Founder, architect, project manager, and lead developer *2021–present*
  - Software for massively parallel generalized many-body expansion and basis-set superposition corrections.
  - Contributions: concept, design, CI infrastructure, initial implementations.
- **CMakePP** https://github.com/CMakePP
  Founder, architect, project manager, and lead developer *2019–present*
  - Object-oriented CMake build system.
  - Contributions: concept, design, CI infrastructure, CMakePP language
  - Software products:
    - CMINX — https://github.com/CMakePP/CMinx
    - CMAKETEST — https://github.com/CMakePP/CMakeTest
    - CMAKEPPLANG — https://github.com/CMakePP/CMinx
    - CMAIZE — https://github.com/CMakePP/CMaize
- **Psi4** https://psicode.org/
  Developer *2014–2017*
  - Electronic structure package focused on providing a user-friendly experience.
  - Contributions: SCF, infrastructure, many-body expansion
- **Q-Chem** https://www.q-chem.com/
  Developer *2008–2013*
  - Commercial electronic structure package focused on good performance on workstations and small clusters.
  - Contributions: QM/MM

Expertise

- **Computational Chemistry Topics:**
  wave function methods, fragment-based methods
- **Productivity Tools:**
  Git, GitHub, VSCode, Slack
- **Computer Languages:**
  C/C++, Python, CMake, LaTeX, Bash
- **Markup Languages:**
  Doxygen, Sphinx-flavored reStructured Text, Markdown
- **Python Packages:**
  Jupyter Notebooks, Matplotlib, Numpy, Sphinx
- **C++ Libraries:**
  Boost, Catch2, Cereal, PyBind11
- **High-Performance Computing Libraries:**
  BLAS, LAPACK, MPI

Honors and Awards

- **Better Scientific Software Fellow** — **BSSw.io**
  Recipient of 1 of 6 BSSw Fellowships — *2024*
  - Recognizes work for promoting better scientific software.
  - Awarded for: Multi-Project CI/CD for modular scientific software
- **Ames National Laboratory Scientist Leadership Development Program** — **Ames, IA**
  Accepted into 2022 – 2023 cohort — *2022 – 2023*
  - Nominees are junior level scientists at the laboratory who show leadership potential.
  - Program focuses on mentoring and developing leadership skills with a focus on career advancement at a Department of Energy National Laboratory.
- **ISU Research Collaboration Catalysts** — **Ames, IA**
  Accepted into 2020 – 2021 cohort — *2020 – 2021*
  - Nominees demonstrate potential to lead future high-impact interdisciplinary research teams.
  - Provided educational opportunities to refine leadership skills.
- **Finalist for the Emerging Technology in Computational Chemistry Symposium** — **Philadelphia,PA**
  252nd American Chemical Society National Meeting and Exposition — *2016*
- **The Ohio State University Graduate School Fellowship** — **Columbus, OH**
  The Ohio State University — *2008–2009*
- **Best Undergraduate Presentation** — **South Euclid, OH**
  Notre Dame College — *2007*
- **Cleveland State University Honors Program Scholarship** — **Cleveland, OH**
  Cleveland State University — *2004–2008*

Active Grants

- **ISU LAS Frontier Science Award** — **Ames, IA**
  Theresa Windus (PI) and Ryan M. Richard *(co-PI)* — *2025–2027*
  Error-Bound Atomistic Simulations for Reliable Machine Learning Models
  Value of award: $100,000.00
- **NSF CHE-2348724** — **Ames, IA**
  Theresa Windus (PI) and Ryan M. Richard *(co-PI)* — *2024–2027*
  REU Site: Sutainability Institute for Machine Learning and Collaborative Open-Source Development of Enzymatic Simulations
  Value of award: $465,000.00

Completed Grants

- **Ames National Laboratory Directed Research and Development FY2025-xxxx-01** — **Ames, IA**
  Ryan M. Richard *(PI)* — *2024–2025*
  Data-Based Approach to Performance and Power Optimization
  Value of award: $250,000.00
- **BSSw Fellowship FY2023-407** — **Ames, IA**
  Ryan M. Richard *(PI)* — *2024–2025*
  Multi-Project CI/CD for Modular Scientific Software
  Value of award: $50,000.00
- **Ames National Laboratory Directed Research and Development FY2024-xxxx-01** — **Ames, IA**
  Ryan M. Richard *(PI)* — *2024*
  Automating Parameter Selection of Fragment Based Methods for Materials Challenges
  Value of award: $287,000.00

- **Ames National Laboratory Directed Research and Development FY2022-xxxx-01** — **Ames, IA**
  Ryan M. Richard *(PI)* — *2021–2022*
  GhostFragment: Making Strong Electron Correlation Less Scary
  Value of award: $48,000.00
- **Renewal of XSEDE Research Allocation number CHE150006** — **Atlanta, GA**
  Ryan M. Richard *(PI), C. D. Sherrill (Co-PI).* — *2016–2017*
  Accurate Crystal Lattice Energies Via Pleasantly Parallel Methods
  Value of award: $115,006.00
- **XSEDE Research Allocation number CHE150006** — **Atlanta, GA**
  Ryan M. Richard *(PI), C. D. Sherrill (Co-PI).* — *2015–2016*
  Applying Quantum Chemistry to Condensed Phase Systems Using the Many-Body Expansion
- **XSEDE Startup Allocation number CHE140145** — **Atlanta, GA**
  Ryan M. Richard *(PI), C. D. Sherrill (Co-PI).* — *2014–2015*
  Accurate Crystal Properties Via Massively Parallel Quantum Chemistry

Professional Service

- **National Laboratory Information Technology (NLIT) Summit**
  Member of the Sustainable Scientific Software (S3C) organizing team. — *2024–2026*
  Helped choose topics for conference and downselect contributed presentations.
- **256th National American Chemical Society Meeting.** — **Boston, MA**
  Session chair — *2018*
- **Article peer review for:**
  Journal of Chemical Physics, Journal of Chemical Theory and Computation
- **Grant reviewer for:**
  Better Scientific Software Fellowship, Lawrence Livermore National Laboratory Computing Grand Challenge

Ames National Laboratory Service

- **Learning Session: AI at the Lab** — **Ames National Laboratory**
  Panelist. — *2024*
  Provided a brief overview of what AI/ML can/cannot do for research and the effort needed to train an AI/ML model.
- **2022 Iowa State Fair** — **Des Moines, IA**
  Ames National Laboratory and Iowa State University Exhibit. — *2022*
  Explained research at Ames National Laboratory to general public and answered questions.
- **Department of Energy's National Science Bowl** — **Ames, IA**
  Moderator and Judge — *2019–Present*
  Helped setup/teardown and served as moderator and judge.

Iowa State University Service

- **Preliminary Examination Committee Member** — **Ames, IA**
  Krishna Suresh (substitute) — *2025*

Georgia Institute of Technology Service

- **PURA (President's Undergraduate Research Award) application reviewer** — **Atlanta, GA**
  Georgia Institute of Technology — *2016*
- **2nd Annual Postdoctoral Research Symposium** — **Atlanta, GA**
  Session chair — *2015*

- **1st Annual Postdoctoral Research Symposium** — **Atlanta, GA**
  Session chair — *2014*
- **'Postdocs@Tech"** — **Atlanta, GA**
  Co-Organizer — *2014–2017*
  Organized monthly social events and an annual university research symposium for postdocs at Georgia Tech.

Students Mentored

Graduate Students

- **Anna Diaz** — **Ames, IA**
  Research focus: uncertainty in eigen solvers, Summer Internship — *2025*
- **Shalith Chamantha** — **Ames, IA**
  Research focus: Quantum chemistry uncertainty propagation — *2024 – Present*
- **Rojas, Felix** — **Ames, IA**
  Research focus: Numerical optimization — *2024 – Present*
- **Heflin, Jacob** — **Ames, IA**
  Research focus: Benchmarking fragment-based methods — *2023 – Present*

Undergraduate Students

- **Daniel Woodard** — **Ames, IA**
  Research focus: predicting fragments of peptides. — *2025*
- **Rishita Kollu** — **Ames, IA**
  Research focus: Designing a composite method library. — *2024*
- **John Lewis** — **Ames, IA**
  Research focus: Benchmarking geometry optimizers. — *2023–Present*
- **Walker Hayes** — **Ames, IA**
  Research focus: Implementing capping methods in GhostFragment — *2023*
- **Issac Van Orman** — **Ames, IA**
  Research focus: Implementing capping methods in GhostFragment — *2023*
- **Theodore Davis** — **Ames, IA**
  Research focus: Object-oriented CMake. — *2020–2021*
- **Emin Okic** — **Ames, IA**
  Research focus: Continuous integration for CMake. — *2020–2021*
- **Allison Finger** — **Ames, IA**
  Research focus: Object-oriented CMake. — *2020*
- **Blake Mulnix** — **Ames, IA**
  Research focus: Object-oriented CMake. — *2020*
- **Jacob Brunton** — **Ames, IA**
  Research focus: Improving self-consistent field guesses. — *2020*
- **Branden Butler** — **Ames, IA**
  Research focus: CMake documentation and unit testing — *2019–Present*
- **Andres Garcia-Alejo** — **Ames, IA**
  Research focus: Machine learning molecular structure — *2018–2019*
- **Brodie Schroeder** — **Ames, IA**
  Research focus: Machine learning applications to quantum chemistry — *2017*
- **Michael Zott** — **Atlanta, GA**
  Research focus: Understanding the many-body expansion — *2015–2017*

Other Mentoring Activities

- **Anna Diaz** — **Ames, IA**
  Graduate Student Summer Internship. Research focus: uncertainty in eigen solvers — *2025*
- **Nancy L. Glenn Griesinger** — **Ames, IA**
  Visiting Faculty Program. Research focus: uncertainty in electron repulsion integrals. — *2025*

Invited Presentations

2025

19. **Ryan M. Richard**. *TensorWrapper Wishful Thinking?*. Toulouse Tensor Workshop. Toulouse, France. August 2025
18. **Ryan M. Richard**. *NWChemEx: Towards a fully reusable electronic structure package*. Majvik, Finland. July 2025

2024

17. **Ryan M. Richard**. *The NWChemEx Community's contributions to performance portable, modular, reusable, and interoperable computational chemistry*. The 75th Southeastern Regional Meeting of the American Chemical Society. Atlanta, GA. October 2024.
16. **Ryan M. Richard**. *PluginPlay: Enabling high- performance scientific software one module at a time*. CECAM Flagship Workshop. Lausanne, Switzerland. February 2024.

2023

15. **Ryan M. Richard**. *NWChemEx: Designing a Computational Chemistry App Store for The Exascale*. APS March Meeting. Las Vegas, NV. March 2023.
14. **Ryan M. Richard**. *NWChemEx: Challenges Faced in Designing an Electronic Structure Program for the Exascale*. SIAM Conference on Computational Science and Engineering. Amsterdam, New Holland. The Netherlands. February 2023.

2022

13. **Ryan M. Richard**. *Software design for the exascale era: The NWChemEx perspective*. 2022 Midwest Regional Meeting for the American Chemical Society. October 2022.

2019

12. **Ryan M. Richard**. *The SDE: A General Computational Chemistry Software Framework*. Blue Waters Webinar. March 2019.
11. **Ryan M. Richard** and Theresa L. Windus. *CMake Packaging Project: Reliable, Reproducible, and Reusable Build Systems Made Easy*. Spring NWChemEx Team Meeting. Richland, WA. March 2019.
10. **Ryan M. Richard**. *The Simulation Development Environment (SDE): A C++ Framework for Reusable Computational Chemistry*. Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering. Spokane, WA. February 2019.

2018

9. **Ryan M. Richard**. *Applying Ab Initio Methods to Large Molecules*. Ames Laboratory. Ames, IA. August 2018.

2017

8. **Ryan M. Richard**. *Exascale Prototyping Via A Computational Chemistry App Store*. 254^{th} National American Chemical Society Meeting. Washington, D.C. August 2017.

2016

7. **Ryan M. Richard**. *Pulsar: A Computational Chemistry App Store*. PSI4 Developers Meeting. University of Georgia. Athens, GA. November 2016.
6. **Ryan M. Richard**. *ForcemanII: Status and Possible Future Directions*. Q-CHEM Developers Meeting. University of Pennsylvania. Philadelphia, PA. August 2016.
5. **Ryan M. Richard**. *Understanding Chemistry Via Fragment Based Methods*. University of Tennessee. Knoxville, TN. February 2016.
4. **Ryan M. Richard**. *Understanding Chemistry Via Fragment Based Methods*. Youngstown State University. Youngstown, OH. February 2016.
3. **Ryan M. Richard**. *Understanding Chemistry Via Fragment Based Methods*. Tennessee Technological University. Cookeville, TN. January 2016.

2015

2. **Ryan M. Richard**. *Understanding Chemistry Via Fragment Based Methods*. University of North Florida. Jacksonville, FL. November 2015.

2008

1. **Ryan M. Richard**, David W. Ball. *Thermodynamic Studies on the Potential Use of Boron- and/or Nitrogen-Containing Molecules as New High Energy Materials*. Ohio State University. Columbus, OH. February 2008.

Contributed Presentations

2025

22. **Ryan M. Richard**. *GhostFragment: a reusable, flexible, modular library for generalized fragment-based methods*. Pacifichem 2025. Honolulu, HI. December 2025.

2019

21. **Ryan M. Richard** and Theresa L. Windus. *CMake Packaging Project: Reliable, Reproducible, and Reusable Build Systems Made Easy*. 257^{th} National American Chemical Society Meeting. Orlando, FL. April 2019.
20. **Ryan M. Richard**, Kristopher Keipert, Thom Dunning Jr., Robert Harrison, and Theresa L. Windus. *The NWChemEx Simulation Development Environment - A General Computational Chemistry Framework*. Poster Presentation. Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering. Spokane, WA. February 2019.

2018

19. **Ryan M. Richard** and Theresa L. Windus. *Leveraging* NWCHEMEX*'s computational chemistry app store to design an exascale SCF*. Oral Presentation. 256^{th} National American Chemical Society Meeting. Boston, MA. August 2018.
18. **Ryan M. Richard**, Brandon W. Bakr, and C. David Sherrill. *Understanding the Many-Body Basis Set Superposition Error: Beyond Boys and Bernardi*. Oral Presentation. 50^{th} Midwest Theoretical Chemistry Conference. Chicago, IL. June 2018.

2017

17. **Ryan M. Richard**. *Leveraging a Computational Chemistry App-Store for Both Teaching and Researching Chemistry*. Oral Presentation. 254^{th} National American Chemical Society Meeting. Washington, D.C. August 2017.

2016

16. **Ryan M. Richard**, Ben Pritchard, and C. D. Sherrill. *Leveraging a Computational Chemistry App Store to Compute High Accuracy Lattice Energies of Molecular Crystals*. Oral Presentation. 252^{nd} American Chemical Society National Meeting and Exposition. Philadelphia, PA. August 2016

15. **Ryan M. Richard**, Brandon Bakr, and C. D. Sherrill. *Understanding Basis Set Superposition Error in Many-Body Systems: Beyond Boys and Bernardi*. Oral Presentation. 47^{th} Southeast Theoretical Chemistry Association Annual Meeting. Tallahassee, FL. May 2016

2015

14. **Ryan M. Richard**, Michael S. Marshall, Jean-Luc Brédas, Noa Marom, and C. D. Sherrill. *CCSD(T)/CBS Benchmark Quality Ionization Potentials (IP) and Electron Affinities (EA)*. Poster Presentation. 2^{nd} Annual Postdoctoral Research Symposium. Atlanta, GA. October 2015.

13. **Ryan M. Richard**, C. D. Sherrill. *Massively Parallel Fragment Based Methods as Implemented in* Psi4. Oral Presentation. 250^{th} American Chemical Society National Meeting and Exposition. Boston, Massachusetts. August 2015.

12. **Ryan M. Richard**, Michael S. Marshall, Jean-Luc Brédas, Noa Marom, and C. D. Sherrill. *CCSD(T)/CBS Benchmark Quality Ionization Potentials (IP) and Electron Affinities (EA)*. Poster Presentation. 46^{th} Southeast Theoretical Chemistry Association Annual Meeting. Orlando, Florida. May 2015.

2014

11. **Ryan M. Richard**, C. D. Sherrill. *Achieving Chemical Understanding Via High Performance Computing*. Oral Presentation. 1^{st} Annual Postdoctoral Research Symposium. Atlanta, Georgia. September 2014.

2013

10. **Ryan M. Richard**, J. M. Herbert. *Achieving the Complete-Basis Limit in Large Molecular Clusters: Computationally Efficient Procedures to Eliminate Basis-Set Superposition Error*. Oral Presentation. 246^{th} American Chemical Society National Meeting and Exposition. Indianapolis, Indiana. September 2013.

9. **Ryan M. Richard**, J. M. Herbert. *Achieving the Complete-Basis Limit in Large Molecular Clusters: Computationally Efficient Procedures to Eliminate Basis-Set Superposition Error*. Oral Presentation. 68^{th} International Symposium on Molecular Spectroscopy. Columbus, Ohio. June 2013.

8. **Ryan M. Richard**, J. M. Herbert. Oral Presentation. 45^{th} Midwest Theoretical Chemistry Conference. Champaign, Illinois. May 2013.

2012

7. **Ryan M. Richard**, J. M. Herbert. *A Generalized Many-Body Expansion and a Unified View of Fragment-Based Methods in Electronic Structure Theory*. Poster presentation. 44^{th} Midwest Theoretical Chemistry Conference. Madison, Wisconsin. June 2012.

2011

6. **Ryan M. Richard**, J. M. Herbert. *TDDFT Calculations of Transient IR Spectra of DNA*. Oral Presentation. 66^{th} International Symposium on Molecular Spectroscopy. Columbus, Ohio. June 2011.

5. **Ryan M. Richard**, J. M. Herbert. *Time-Dependent Density- Functional Description of the ^1L_a State in Polycyclic Aromatic Hydrocarbons: Charge-Transfer State in Disguise?*. Poster Presentation. 43^{rd} Midwest Theoretical Chemistry Conference. South Bend, Indiana. June 2011.

2010

4. **Ryan M. Richard**, J. M. Herbert. *Determination of Exciton Length in Aqueous B-DNA Using Long-Range Time-Dependent Density Functional Theory (LRC-TDDFT)*. Oral Presentation. 65^{th} International Symposium on Molecular Spectroscopy. Columbus, Ohio, June 2010.

2008

3. **Ryan M. Richard**, D. W. Ball. *Thermodynamic Studies on Boron and Nitrogen Containing Spiropentanes*. Oral Presentation. American Chemical Society Meeting in Miniature. Oberlin College. Oberlin, OH. March 2008.

2007

2. **Ryan M. Richard**, D. W. Ball. *G2, G3, and Complete Basis Set Calculations on Small Hydroboranes and Mixed Boron-Nitrogen Containing Rings*. American Chemical Society Meeting in Miniature. Notre Dame College. South Euclid, OH. March 2007. Winner of Best Undergraduate Presentation.

1. **Ryan M. Richard**, D. W. Ball. *New Potential High Energy Materials*. Cleveland State University Undergraduate Research Symposium. Summer 2007

Miscellaneous Workshops and Presentations

2. Organizer for Virtual Workshop on Multi-Project CI/CD. Virtual. 2024.

1. **Ryan M. Richard**. *Best Practices for Multi-project CI/CD*. NLIT (National Laboratory Information Technology) Summit 2024. Seattle, Washington. April 2024.

Non Peer-Reviewed Publications

3. **Ryan M. Richard**. *Best Practices for Multi-Project Continuous Integration and Deployment*.`https://bssw.io/blog_posts/best-practices-for-multi-project-continuous-integration-and-deployment`.

2. **Ryan M. Richard**, T. L.Windus. *Is a Language Barrier Impeding Development of Better Scientific Software?*. ASCR (Advanced Scientific Computing Research) Workshop on the Science of Scientific-Software Development and Use. Virtual. December 13-15 2021.

1. **Ryan M. Richard**, Z. Crandall, H. v. Dam, N. Govind, K. Kowalski, T. L. Windus. Stewardship of Software for Scientific and High-Performance Computing. Office of Advanced Scientific Computing Research.

Review Articles

2. **Ryan M. Richard**, K. U. Lao, J. M. Herbert. *Aiming for Benchmark Accuracy with the Many-Body Expansion*. Accounts of Chemical Research. 47 (2014) 2828-2836.

1. L. D. Jacobson, **Ryan M. Richard**, K. U. Lao, J. M. Herbert. *Efficient Monomer-Based Quantum Chemistry Methods for Molecular and Ionic Clusters*. Annual Reports of Computational Chemistry. 9 (2013) 25-56.

Publications

2025

39. K. Fujioka, **Ryan M. Richard**, J. Waldrop, Y. Lou, T. L. Windus, and R. Sun. *VENUSpy: A Chemical Dynamics Simulation Program in the Era of Machine Learning and Exascale Computing*. Journal of Chemical Theory and Computation. 21 (2025) 10679.

38. J. M. Waldrop, W. de Jong, E. F. Valeev, T. L. Windus, and **Ryan M. Richard**. *Chemist: A Domain-Specific Language by Chemists for Chemists*. The Journal of Physical Chemistry A. 129 (2025) 7964.

37. C. Stevens, K. Kjeer, **Ryan M. Richard**, E. Valeev, M. Cohen. *Model Assisted Refinement of Metamorphic Relations for Scientific Software*. ICSE 2025 New Ideas and Emerging Results (Conference Proceeding).

36. J. M. Waldrop, **Ryan M. Richard**. *Sigma: Uncertainty Propagation for C++*. Journal of Open Source Software. 10 (2025) 7404.

2024

35. Z. Crandall, T. L. Windus, **Ryan M. Richard**. *CMaize: Simplifying inter-package modularity from the build up.*Journal of Chemical Physics. 160 (2024) 092502.

2023

34. V. Gavini . . . **Ryan M Richard**. . . D. Perez. *Roadmap on electronic structure codes in the exascale era*. Modelling and Simulation in Materials Science and Engineering. 31 (2023) 063301. (30^{th} author of 41)

33. **Ryan M. Richard**, K. Keipert, J. Waldrop, M. Keçeli, D. Williams-Young, R. Bair, J. Boschen, Zachery Crandall, Kevin Gasperich, Quazi Ishtiaque Mahmud, A. Panyala, E. Valeev, H. van Dam, W A. de Jong, T. L. Windus. *PluginPlay: Enabling exascale scientific software one module at a time*. The Journal of Chemical Physics. 158 (2023) 184801.

2022

32. B. Butler and **Ryan M. Richard**. *CMinx: A CMake Documentation Generator*. Journal of Open Source Software. 7 (2022) 4680.

2021

31. E. Epifanovsky, . . ., **Ryan M. Richard**, . . ., A. I. Krylov. *Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package*. The Journal of Chemical Physics. 155 (2021) 084801. (139^{th} of 220 authors).

30. Karol Kowalski, . . ., **Ryan M. Richard**, . . ., Theresa L. Windus. *From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape*. Chemical Reviews. 121 (2021) 4962- 4998. (19th of 29 authors).

2020

29. Edoardo Apra, . . ., **Ryan Richard**, . . ., and Robert Harrison . *NWChem: Past, Present, and Future*. Journal of Chemical Physics. 152 (2020) 184102. (82^{nd} of 114 authors).

2019

28. **Ryan M. Richard**, Colleen Bertoni, Jeffery S. Boschen, Kristopher Keipert, Benjamin Pritchard, Edward F. Valeev, Robert J. Harrison, Wibe A. de Jong, and Theresa L. Windus. *Developing a Computational Chemistry App Store for the Exascale Era*. Computing in Science & Engineering. 21 (2019) 48.

2018

27. **Ryan M. Richard**, Brandon Bakr, and C. David Sherrill. *Understanding the Many-Body Basis Superposition Error: Beyond Boys and Bernardi*. Journal of Chemical Theory and Computation. 14 (2018) 2386.

2017

26. Robert M. Parrish, . . .,**Ryan M. Richard**, . . . *Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability*. Journal of Chemical Theory and Computation. 13 (2017) 3185. (10^{th} of 26 authors)

2016

25. Ka Un Lao , Kuan-Yu Liu ,**Ryan M. Richard** , and John M. Herbert. *Understanding the many-body expansion for large systems. II. Accuracy considerations.* Journal of Chemical Physics. 144 (2016) 164105.

24. O. Dolgounitcheva, Manuel Díaz–Tinoco, V. G. Zakrzewski, **Ryan M. Richard**, Noa Marom, C. David Sherrill and J. V. Ortiz. *Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron–Propagator Methods*. Journal of Chemical Theory and Computation. 12 (2016) 627-637.

23. **Ryan M. Richard**, Michael S. Marshall, Olga Dolgounitcheva, J. V. Ortiz, Jean-Luc Brédas, Noa Marom, and C. David Sherrill. *Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules. I. Reference Data at the CCSD(T) Complete Basis Set Limit.* Journal of Chemical Theory and Computation. 12 (2016) 595-604.

2015

22. Y. Shao, ..., **Ryan M. Richard**,... *Advances in Molecular Quantum Chemistry Contained in the Q-Chem 4 Program Package*. Molecular Physics. 113 (2015) 184-215. (22^{nd} author out of 150).

2014

21. **Ryan M. Richard**, K. U. Lao, J. M. Herbert. *Understanding the Many-Body Expansion for Large Systems. I. Precision Considerations*. The Journal of Chemical Physics. 141 (2014) 014108:1-14.

2013

20. Z. C. Holden, **Ryan M. Richard**, J. M. Herbert. *Periodic Boundary Conditions for QM/MM Calculations: Ewald Summation for Extended Gaussian Basis Sets*. The Journal of Chemical Physics. 139 (2013) 244108:1-13.

19. **Ryan M. Richard**, K. U. Lao, J. M. Herbert. *Approaching the Complete-Basis Limit with a Truncated Many-Body Expansion*. The Journal of Chemical Physics. 139 (2013) 224102:1-11.

18. **Ryan M. Richard**, K. U. Lao, J. M. Herbert. *Achieving the CCSD(T) Basis-Set Limit in Sizable Molecular Clusters: Counterpoise Corrections for the Many-Body Expansion*. The Journal of Physical Chemistry Letters. 4 (2013) 2674-2680.

17. **Ryan M. Richard**, J. M. Herbert. *Many-Body Expansion with Overlapping Fragments: Analysis of Two Approaches*. Journal of Chemical Theory and Computation. 9 (2013) 1408-1416.

2012

16. **Ryan M. Richard**, J. M. Herbert. *A Generalized Many-Body Expansion and a Unified View of Fragment-Based Methods in Electronic Structure Theory*. The Journal of Chemical Physics. 137 (2012) 064113.

15. W. Morales, K. W. Street Jr., **Ryan M. Richard**, D. J. Valco. *Tribological Testing and Thermal Analysis of an Alkyl Sulfate Series of Ionic Liquids for Use as Aerospace Lubricants*. Tribology Transactions. 55 (2012) 815-821.

2011

14. K. W. Street Jr., W. Morales, V. R. Koch, D. J. Valco, **Ryan M. Richard**, N. Hanks. *Evaluation of Vapor Pressure and Ultra-High Vacuum Tribological Properties of Ionic Liquids*. Tribology Transactions. 54 (2011) 911-919.

13. **Ryan M. Richard**, J. M. Herbert. *Time-Dependent Density- Functional Description of the ^1L_a State in Polycyclic Aromatic Hydrocarbons: Charge-Transfer Character in Disguise?* Journal of Chemical Theory and Computation. 7 (2011) 1296-1306.

2009

12. **Ryan M. Richard**, D. W. Ball. *B3LYP Calculations on the Thermodynamic Properties of a Series of Nitroxycubanes Having the Formula $C_8H_{8-x}(NO_3)_x$ (x=1–8)*. Journal of Hazardous Materials. 164 (2009) 1593-1600.

11. **Ryan M. Richard**, D. W. Ball. *Density Functional Calculations on the Thermodynamic Properties of a Series of Nitrosocubanes Having the Formula $C_8H_{8-x}(NO)_x$ (x=1–8)*. Journal of Hazardous Materials. 164 (2009) 1552-1555.

2008

10. **Ryan M. Richard**, D. W. Ball. *Ab Initio Calculations on the Thermodynamic Properties of Azaspiropentanes*. The Journal of Physical Chemistry A. 112 (2008) 2618-2627.
9. **Ryan M. Richard**, D. W. Ball. *Enthalpies of Formation of Nitrobuckminsterfullerenes: Extrapolation to $C_{60}(NO_2)_{60}$*. Journal of Molecular Structure: THEOCHEM. 858 (2008) 85-87.
8. **Ryan M. Richard**, D. W. Ball. *Ab Initio Calculations on the Thermodynamic Properties of Spiropentane and its Boron-Containing Derivatives*. Journal of Molecular Structure: THEOCHEM. 851 (2008) 284-293.
7. **Ryan M. Richard**, D. W. Ball. *Ab Initio Calculations on the Thermodynamic Properties of Azaborospiropentanes*. Journal of Molecular Modeling. 14 (2008) 871-878.
6. **Ryan M. Richard**, D. W. Ball. *G2, G3, and Complete Basis Set Calculations on the Thermodynamic Properties of Triazane*. Journal of Molecular Modeling. 14 (2008) 29-37.
5. **Ryan M. Richard**, D. W. Ball. *G2, G3, and Complete Basis Set Calculations of the Thermodynamic Properties of Cis- and Trans- Triazene*. Journal of Molecular Modeling. 14 (2008) 21-27.

2007

4. **Ryan M. Richard**, D. W. Ball. *G2, G3, and Complete Basis Set Calculations of the Thermodynamic Properties of Aminoborane, Diaminoborane, and Triaminoborane*. Journal of Molecular Structure: THEOCHEM. 823 (2007) 6-15.
3. **Ryan M. Richard**, D. W. Ball. *B3LYP, G2, G3 and Complete Basis Set Calculations of the Thermodynamic Properties of Small Cyclic and Chain Hydroboranes*. Journal of Molecular Structure: THEOCHEM. 814 (2007) 91-98.
2. **Ryan M. Richard**, D. W. Ball. *G2, G3, and Complete Basis Set Calculations of Optimized Geometries, Vibrational Frequencies, and Thermodynamic Properties of Azatriboretidine and Triazaboretidine*. Journal of Molecular Structure: THEOCHEM. 806 (2007) 165-170.
1. **Ryan M. Richard**, D. W. Ball. *Optimized Geometries, Vibrational Frequencies, and Thermochemical Properties of Mixed Boron- and Nitrogen-Containing Three-Membered Rings*. Journal of Molecular Structure: THEOCHEM. 806 (2007) 113-120.

2006

0. **Ryan M. Richard**, D. W. Ball. *G2, G3, and Complete Basis Set Calculations of the Thermodynamic Properties of Boron-Containing Rings: cyclo-CH_2BHNH, 1,2-, and 1,3-cyclo-C_2H_4BHNH*. Journal of Molecular Structure: THEOCHEM. 776 (2006) 89-96.