

# Ryan M. Richard — Chemistry

Ames National Laboratory and Iowa State University – Ames, IA – USA

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🌐 <https://rmrresearch.github.io/>

Scientist II 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

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- **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

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- **Scientist II, Ames National Laboratory** **Ames, IA**  
Architect and a 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

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- **Adjunct Assistant Professor of Chemistry, Iowa State University** **Ames, IA**  
High-accuracy benchmark development. 2022–Present  
Additional Responsibilities: Co-advise graduate students.
- **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 benchmarking 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

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- **NWChemEx** <https://github.com/NWChemEx-Project>  
*Architect and lead developer* 2017–present
  - Package focused on high-performance, massively parallel electronic structure theory.
  - Contributions: design, plugin framework, CI infrastructure, SCF, MP2, MP2-F12, CCSD-F12
- **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
- **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

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- **Computational Chemistry Topics:**  
Hartree-Fock, MP2, coupled-cluster, explicit correlation, domain-local methods, fragment-based methods
- **Productivity Tools:**  
Git, GitHub, VSCode, Slack
- **Computer Languages:**  
C/C++, Python, CMake, L<sup>A</sup>T<sub>E</sub>X, 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

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- **Better Scientific Software Fellow** [BSSw.io](https://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**  
*252<sup>nd</sup> 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*

## Professional Service

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- **Virtual Workshop on Multi-Project CI/CD** **Virtual**  
*Organizer and moderator.* *2024*  
 Workshop sought to create a community of practice for DevOps professionals managing CI/CD workflows for multiple software project.
- **National Laboratory Information Technology (NLIT) Summit 24** **Seattle, WA**  
*Member of the Sustainable Scientific Software (S3C) organizing team.* *2024*  
 Helped choose topics for conference and downselect contributed presentations.
- **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.
- **256<sup>th</sup> National American Chemical Society Meeting.** **Boston, MA**  
*Session chair* *2018*
- **PURA (President's Undergraduate Research Award) application reviewer** **Atlanta, GA**  
*Georgia Institute of Technology* *2016*
- **2<sup>nd</sup> Annual Postdoctoral Research Symposium** **Atlanta, GA**  
*Session chair* *2015*
- **1<sup>st</sup> 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.
- **Peer Reviewer for:**  
*Journal of Chemical Physics, Journal of Chemical Theory and Computation*

## Active Grants

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- **NSF CHE-2348724** **Ames, IA**  
*Theresa Windus (PI) and Ryan M. Richard (co-PI)* *2024–2027*  
 REU Site: Sustainability Institute for Machine Learning and Collaborative Open-Source Development of Enzymatic Simulations  
 Value of award: \$465,000.00

- **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
- **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

## Completed Grants

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- **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

## Students Mentored

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### Graduates.....

- **Heflin, Jacob** **Ames, IA**  
*Research focus: Benchmarking fragment-based methods* 2023 – Present

### Undergraduates.....

- **Lewis, John** **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**  
2019–Present  
Research focus: CMake documentation and unit testing
- **Andres Garcia-Alejo** **Ames, IA**  
2018–2019  
Research focus: Machine learning molecular structure
- **Brodie Schroeder** **Ames, IA**  
2017  
Research focus: Machine learning applications to quantum chemistry
- **Michael Zott** **Atlanta, GA**  
2015–2017  
Research focus: Understanding the many-body expansion

## Invited Presentations

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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<sup>th</sup> National American Chemical Society Meeting. Washington, D.C. August 2017.

2016.....

7. **Ryan M. Richard.** *Pulsar: A Computational Chemistry App Store.* PS14 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

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- 2019.....
21. **Ryan M. Richard** and Theresa L. Windus. *CMake Packaging Project: Reliable, Reproducible, and Reusable Build Systems Made Easy.* 257<sup>th</sup> 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<sup>th</sup> 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<sup>th</sup> 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<sup>th</sup> 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<sup>nd</sup> 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<sup>th</sup> 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<sup>nd</sup> 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<sup>th</sup> 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<sup>th</sup> 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<sup>st</sup> 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<sup>th</sup> 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<sup>th</sup> International Symposium on Molecular Spectroscopy. Columbus, Ohio. June 2013.
8. **Ryan M. Richard**, J. M. Herbert. Oral Presentation. 45<sup>th</sup> 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<sup>th</sup> 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<sup>th</sup> 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<sup>rd</sup> 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<sup>th</sup> 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

## Birds of a Feather Sessions

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

## Position Papers

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1. **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.

## Request for Information

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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

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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

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2024.....

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

2023.....

35. 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<sup>th</sup> author of 41)
34. **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.....

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



## 2021.....

32. 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<sup>th</sup> of 220 authors).
31. Karol Kowalski, ..., **Ryan M. Richard**, ..., Theresa L. Windus. *From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape*. Chemical Reviews. 121 (2021) 4962- 4998. (19<sup>th</sup> of 29 authors).

## 2020.....

30. Edoardo Apra, ..., **Ryan Richard**, ..., and Robert Harrison . *NWChem: Past, Present, and Future*. Journal of Chemical Physics. 152 (2020) 184102. (82<sup>nd</sup> of 114 authors).

## 2019.....

29. **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.....

28. **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.....

27. 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<sup>th</sup> of 26 authors)

## 2016.....

26. 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.
25. 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.
24. **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.....

23. 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<sup>nd</sup> author out of 150).

## 2014.....

22. **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.....

21. 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.

20. **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.
  19. **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.
  18. **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.....
17. **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.
  16. 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.....
15. 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.
  14. **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.....
13. **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.
  12. **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.....
11. **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.
  10. **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.
  9. **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.
  8. **Ryan M. Richard**, D. W. Ball. *Ab Initio Calculations on the Thermodynamic Properties of Azaborospiropentanes*. Journal of Molecular Modeling. 14 (2008) 871-878.
  7. **Ryan M. Richard**, D. W. Ball. *G2, G3, and Complete Basis Set Calculations on the Thermodynamic Properties of Triazene*. Journal of Molecular Modeling. 14 (2008) 29-37.
  6. **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.....

5. **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.
4. **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.
3. **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.
2. **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.....

1. **Ryan M. Richard**, D. W. Ball. *G2, G3, and Complete Basis Set Calculations of the Thermodynamic Properties of Boron-Containing Rings: cyclo-CH<sub>2</sub>BH<sub>2</sub>NH, 1,2-, and 1,3-cyclo-C<sub>2</sub>H<sub>4</sub>BH<sub>2</sub>NH*. Journal of Molecular Structure: THEOCHEM. 776 (2006) 89-96.