Kurt R. Brorsen

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Professional Experience

Assistant Professor August 2018 – Present
Department of Chemistry, University of Missouri

Postdoctoral Researcher June 2014 – July 2018
Department of Chemistry, University of Illinois-Urbana Champaign
Advisor: Sharon Hammes-Schiffer

Education

Ph.D. in Physical Chemistry May 2014
Iowa State University
Advisor: Mark S. Gordon

B.S. in Chemistry and B.S. in Mathematics May 2008
University of Oklahoma

Peer-Reviewed Publications
University of Missouri

29. Samsonova, I.; Tucker, G.; Alaal, N.; Brorsen, K.R. Electronic Basis Sets for Multicomponent Computational Chemistry Calculations *ACS Omega* **2023** 8 (5) 5033

28. Wyatt, Q.; Brathwaite, K.; Ardiansyah, M.; Paranamana, N.; Brorsen. K.R.; Young, M.Y. Mechanistic Insights into Oxidative Molecular Layer Deposition of Conjugated Polymers. *Chem. Mat.* **2023** 35 (1) 154.

27. Fowler, D.; Brorsen, K.R. A (T) Correction for Multicomponent Coupled-Cluster Theory. *J. Chem. Theory Comput.* **2022** 18 (12) 7298.

26. Gettler, R.; Alaal, N.; Brorsen, K.R.; Young, M.Y. Effects of Interchain Crosslinking by Alkyl Dihalides on the Electrochemical Performance of Nanoscale Polypyrrole Films. *Chem. Mat.* **2022** 34 (17) 8065.

25. Allal, N; Brorsen, K.R. Multicomponent Heat-Bath Configuration Interaction with the Perturbative Correction for the Calculation of Protonic Excited States. *J. Chem. Phys.* **2021**. 155 (24) 234107.

24. Fajen, O.J.; Brorsen, K.R. Multicomponent MP4 and the Inclusion of Triple excitations in Multicomponent Many-Body Methods. *J. Chem. Phys.* **2021**. 155 (24) 234108.

23. Bhatty, A.U.; Brorsen, K.R. An Alternative Formulation of Vibrational Heat-Bath Configuration Interaction. *Mol. Phys.* **2021**. *E1936250*.

22. Fajen, O.J.; Brorsen, K.R. Multicomponent CASSCF Revisited: Large Active Spaces are needed for Qualitatively Accurate Protonic Densities. *J. Chem. Theory Comput.* **2021**. 17, (2) 965.

21. Ardiansyah, M.; Brorsen, K.R. Quantum-Classical Dynamics with Machine Learning-Based Potentials via Wigner Sampling. *J. Phys. Chem. A* **2020**. 24, (44) 9326.

20. Fajen, O.J.; Brorsen, K.R. Separation of Electron-Electron and Electron-Proton Correlation in Multicomponent Orbital-Optimized Perturbation Theory. *J. Chem. Phys.* **2020.** 152. (19), 194107.

19. Brorsen, K.R. Quantifying Multireference Character of Multicomponent Systems with Heat-Bath Configuration Interaction. *J. Chem. Theory Comput.* **2020**, 16, (4), 2379.

18. Lesko, E.; Ardiansyah, M.; Brorsen, K.R. Vibrational Adaptive Sampling Configuration Interaction. *J. Chem. Phys.* **2019**, 151, (16). 164103.

17. Brorsen, K.R. Reproducing Global Potential Energy Surfaces with Continuous-Filter Convolutional Neural Networks. *J. Chem. Phys.* **2019**, 150 (20), 204104.

Prior to University of Missouri

16. Brorsen, K.R.; Schneider, P.E., Hammes-Schiffer, S. Alternative Forms and Transferability of Electron-Proton Correlation Functionals in Nuclear-Electronic Orbital Density Functional Theory. *J. Chem. Phys.* **2018**, 149 (4), 044110.

15. Yang, Y.; Brorsen, K.R.; Pak, M.V.; Culpitt, T.; Hammes-Schiffer, S. Development of a Practical Multicomponent Density Functional for Electron-Proton Correlation to Produce Accurate Proton Densities. *J. Chem. Phys.* **2017**, *147* (11), 114113

14. Brorsen, K.R.; Yang, Y.; Hammes-Schiffer, S. Multicomponent Density Functional Theory: Impact of Nuclear Quantum Effects on Proton Affinities and Geometries. *J. Phys. Chem. Lett.* **2017**, *8 (15)*, 3488-3493.

13. Culpitt, T.; Brorsen, K.R.; Hammes-Schiffer, S. Density Theory Embedding with the Orthogonality Constrained Basis Set Expansion Procedure. *J. Chem. Phys.* **2017**, *146* (21), 211101.

12. Brorsen, K. R.; Yang, Y.; Pak, M.V.; Hammes-Schiffer, S. Is the Accuracy of Density Functional Theory for Atomization Energies and Densities in Bonding Regions Correlated? *J. Phys. Chem. Lett.* **2017**, *8* (9), 2076-2081.

11. Brorsen, K. R.; Pak, M.V.; Hammes-Schiffer, S. Calculation of Positron Binding Energies and Electron-Positron Annihilation Rates for Atomic Systems with the Reduced Explicitly Correlated Hartree-Fock Method in the Nuclear-Electronic Orbital Framework. *J. Phys. Chem. A.* **2016**, *121* (2), 515-522.

10. Culpitt, T.; Brorsen, K. R.; Pak, M. V.; Hammes-Schiffer, S. Multicomponent Density Functional Theory Embedding Formulation. *J. Chem. Phys.* **2016**, *145* (4), 044106.

9. Brorsen, K. R.; Sirjoosingh, A.; Pak, M. V.; Hammes-Schiffer, S. Nuclear-Electronic Orbital Reduced Explicitly Correlated Hartree-Fock Approach: Restricted Basis Sets and Open-Shell Systems. *J. Chem. Phys.* **2015**, *142* (21), 214108.

8. Sirjoosingh, A.; Pak, M. V.; Brorsen, K. R.; Hammes-Schiffer, S. Quantum Treatment of Protons with the Reduced Explicitly Correlated Hartree-Fock Approach. *J. Chem. Phys.* **2015**, *142* (21), 214107.

7. Pruitt, S. R.; Brorsen, K. R.; Gordon, M. S. Ab Initio Investigation of the Aqueous Solvation of the Nitrate Ion. *Phys. Chem. Chem. Phys.* **2015**, *17* (40), 27027-27034.

6. Brorsen, K. R.; Willow, S. Y.; Xantheas, S. S.; Gordon, M. S. The Melting Temperature of Liquid Water with the Effective Fragment Potential. *J. Phys. Chem. Lett.* **2015**, *6* (18), 3555-3559.

5. Pruitt, S. R.; Bertoni, C.; Brorsen, K. R.; Gordon, M. S. Efficient and Accurate Fragmentation Methods. *Acc. Chem. Res.* **2014**, *47* (9), 2786-2794.

4. Brorsen, K. R.; Zahariev, F.; Nakata, H.; Fedorov, D. G.; Gordon, M. S. Analytic Gradient for Density Functional Theory Based on the Fragment Molecular Orbital Method. *J. Chem. Theory Comput.* **2014**, *10* (12), 5297-5307.

3. Brorsen, K. R.; Pruitt, S. R.; Gordon, M. S. Surface Affinity of the Hydronium Ion: the Effective Fragment Potential and Umbrella Sampling. *J. Phys. Chem. B* **2014**, *118* (49), 14382-14387.

2. Brorsen, K. R.; Minezawa, N.; Xu, F.; Windus, T. L.; Gordon, M. S. Fragment Molecular Orbital Molecular Dynamics with the Fully Analytic Energy Gradient. *J. Chem. Theory Comput.* **2012**, *8* (12), 5008-5012.

1. Nagata, T.; Brorsen, K. R.; Fedorov, D. G.; Kitaura, K.; Gordon, M. S. Fully Analytic Energy Gradient in the Fragment Molecular Orbital Method. *J. Chem. Phys.* **2011**, *134* (12), 124115.

Oral Presentations

University of Missouri

28. *Title TBD*, Iowa State University, Ames, IA. November 2024

27. *Title TBD,* Truman State University, Kirksville, MO. September 2024

26. Computing Vibrationally Averaged Properties with Multicomponent Methods, University of Wisconsin-Madison, Madison, WI. February 2024

25. Computing Vibrationally Averaged Properties with Multicomponent Methods, Missouri State University, Springfield, MO. November 2023.

24. Computing Vibrationally Averaged Properties with Multicomponent Methods, American Chemical Society Midwest Regional Meeting, St. Charles, MO. October 2023.

23. Computing Vibrationally Averaged Properties with Multicomponent Methods, University of Oklahoma, Norman, OK. September 2023.

22. Computing Nuclear Quantum Effects with Multicomponent Methods, University of Northern Illinois, DeKalb, IL. April 2023.

21. Many-Body Multicomponent Methods. Kansas State University, Manhattan, KS. March 2023

20. Many-Body Multicomponent Methods, University of Kansas, Lawrence, KS. March 2023.

19. Many-Body Multicomponent Methods. Syracuse University, Syracuse, NY. February 2023

18. Integrating Undergraduates into Computational Chemistry Research. Computational Infusion for Missouri Undergraduate and Science Education Workshop, MORENet Consortium Columbia, MO. August 2022.

17. Inclusion of Connected Triples in Many-Body Multicomponent Methods. 2022 Meeting of the World Association of Theoretical and Organic Chemists, Vancouver, BC. July 2022.

16. Including Nuclear Quantum Effects in Computational Chemistry Calculations with Multicomponent Methods. University of Nebraska-Omaha. April 2022 (Virtual)

15. Considering Multicomponent Methods as Hybrid QM/QM Methods. Spring ACS Meeting, San Diego, CA. March 2022

14. Multicomponent Many-Body Methods and the Importance of Triple Excitations. ACS Midwest Regional Meeting. Springfield, MO. October 2021.

13. Including Select Nuclear Quantum Effects in *Ab Initio* Calculations with Multicomponent Methods. New Frontiers in Electron Correlation. Telluride, CO. June 2021 (Virtual)

12. Towards the Accurate Calculation of Vibrational Excitations of Polycyclic Aromatic Hydrocarbons. Illinois State University, Normal, IL. November 2019.

Prior to the University of Missouri

11. Calculating Electron and Nuclear Densities with Density Functional Theory. Mississippi State University, Starkville, MS. January 2017.

10. Calculating Electron and Nuclear Densities with Density Functional Theory. University of Missouri. Columbia, MO. January 2017.

9. Calculating Electron and Nuclear Densities with Density Functional Theory. Baylor University. Waco, TX. December 2017.

8. Calculating Electron and Nuclear Densities with Density Functional Theory. Texas A&M University. College Station, TX. December 2017

7. Calculating Electron and Nuclear Densities with Density Functional Theory. University of Mississippi, Oxford, MS. December 2017

6. Colle-Salvetti Based Functional for the Inclusion of Electron-Proton Correlation in Multicomponent Density Functional Theory. Fall ACS National Meeting. Washington D.C. August 2017.

5. Is the Accuracy of Density Functional Theory for Atomization Energies and Densities in Bonding Regions Correlated? Blue Waters Symposium. Sunriver, OR. May 2017.

4. Reduced Explicitly Correlated Hartree-Fock in the Nuclear Electronic Orbital Framework Applied to Positronic Atoms. Blue Waters Symposium, Sunriver, OR. June 2016.

3. Quantum Treatment of Protons with the Nuclear Electronic Orbital Method. Blue Waters Symposium. Sunriver, OR. May 2015.

2. Reducing the Nonlinear Scaling of Quantum Chemistry with the Fragment Molecular Orbital Method. Computational Science Graduate Fellowship Program Review. Washington D.C. June 2013.

1. Analytic Gradient for the Fragment Molecular Orbital Method. Spring ACS National Meeting. Anaheim, CA. April 2011.

Student Supervised at the University of Missouri

Graduate Students

7. Colin Gopaul (1st Year; Joint Advised with Matthias Young)
6. Mary Richardson (1st Year)
5. Nazifa Tabassum (2nd Year)
4. Yussuf Fasasi, M.S. 2023;
3. Gabrielle Tucker (3rd Year)
2. Ethan Lesko, M.S. 2022
1. Muhammad Ardiansyah Ph.D. 2023

Postdoctoral Researchers

1. Dr. Naresh Alaal (2021-2023)

Undergraduate Researchers

10. Austin Richards (2024-Present)
9. Matthew Cremer (2023-Present)
8. Dylan Fowler (2021-Present); Goldwater Scholar
7. Gabrielle Tucker (2021); Steven's Scholar Program; Chemistry Graduate Student at University of Missouri
6. Irina Samsonova (2020-2023); Undergraduate Student at University of Missouri
5. Jonathan Fajen (2019-2021); Goldwater Scholar; Chemistry Graduate Student at Stanford University
4. Abuzar Bhatty (2019-2020); Bioinformatics Graduate Student at University of Maryland
3. Ethan Lesko (2019); Steven's Scholar Program; Chemistry Graduate Student at University of Missouri
2. David Peana (2018-2019); Chemistry Graduate Student at Purdue University
1. Alex Roush (2018); High School Math Teacher

High-School Researchers

1. Matthew Cremer (2022-2023); Undergraduate at the University of Missouri

Classes Taught (overall student evaluation scores in parentheses; evaluation metrics changed in Fall 2023)

CHEM1320H Honors College Chemistry I: Fall 2021 (4.59/5.00)
CHEM3700W Undergraduate Seminar – Writing Intensive: Spring 2022 (4.48/5.00)
CHEM4330 Physical Chemistry II: Spring 2020 (4.09/5.00), Spring 2021 (4.82/5.00), Spring 2024 (4.77/5.00)
CHEM8310 Quantum Chemistry: Fall 2018 (N/A), Fall 2020 (4.97/5.00), Fall 2022 (4.63/5.00), Fall 2023 (4.51/5.00)
CHEM8330 Computational Chemistry: Fall 2019 (4.80/5.00)

Grants and Funding

2. Agency: National Science Foundation
   Title: Calculating Molecular Properties with Multicomponent Methods
   Role: Principal Investigator
   Year: 2024-2027
   Amount: $510,00 (KRB share: 100%)

1. Agency: Air Force Office of Scientific Research
   Title: Theoretical and Experimental Investigations of Gas-Phase Molecular Polaritons
   Role: Principal Investigator
   Co-Investigator: Arthur Suits
   Year: 2024-2027
   Amount: $600,000 (KRB share: 80%)

Other Synergistic Activities at the University of Missouri

1. Reviewer for *Journal of Physical Chemistry Letters*, *Journal of Chemical Theory and Computation*, *Chemical Reviews*, *The Journal of Chemical Physics, Journal of Physical Chemistry A, Chem, Computational and Theoretical Chemistry, Molecular Simulation, Molecular Physics, Artificial Intelligence Chemistry*

2. Merit reviewer for the Department of Energy FOA: Scientific Machine Learning and Artificial Intelligence: Uncertainty Quantification. 2019; American Chemical Society: Petroleum Research Fund 2020; Department of Energy: Office of Science Graduate Student Research Program 2020; Department of Energy FOA: Early Career Research Program 2021; DOE-BES Core Research Program 2022; DOE-BES Core Research Program 2023

3. Secretary-Treasurer of Local Section of the American Chemical Society. Columbia, MO. 2019-Present.

4. ACS Symposium Organizer: *Recent Theoretical Progress in Coupled Quantum Systems*. PHYS Division. 2024 Spring ACS Meeting. Denver, CO.

5. ACS Meeting Program Co-Chair. 2025 ACS Midwest Regional Meeting. Columbia, MO.

6. Participant and Speaker – 1st Annual Computational Infusion for Missouri Undergraduate and Science Education Workshop. 2022.

7. Departmental Committees – Graduate Recruitment Committee 2019-2021; Colloquium Committee 2021-Present (Chair 2021-2022)

Awards and Fellowships

Ann K. Covington Award 2023
Outstanding Undergraduate Mentorship at the University of Missouri (Campus Award)

Lindau Fellowship 2010
Department of Energy

Computational Science Graduate Fellowship 2009-2013
Department of Energy

Barry M. Goldwater Fellowship 2007