Samuel J. Stoneburner

Curriculum vitae

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EDUCATION:

- **Doctor of Philosophy in Chemistry,** June 2019, University of Minnesota – Twin Cities, Minneapolis, Minnesota, Gagliardi research group.
- **Master of Science in Chemistry**, January 2016, University of Minnesota – Twin Cities, Minneapolis, Minnesota.
- **Bachelor of Science in Chemistry and Mathematics**, May 2014, Hillsdale College, Hillsdale, Michigan.
- **Associate of Applied Science in Chemical Technology**, May 2010, Kalamazoo Valley Community College, Kalamazoo, Michigan.

TEACHING:

- 2022–Present. Assistant Professor of Chemistry, Point Loma Nazarene University
- 2019–2022. Visiting Assistant Professor of Chemistry, Messiah University
    - Physical Chemistry and General Chemistry lecture and lab courses, including online-only and hybrid online/in-person delivery.
- 2019–2021. Scientific Coordinator, Summer Undergraduate Research Fellowship in Computational and Theoretical Chemistry, University of Minnesota – Twin Cities.
    - Delivered and scheduled training for fellowship recipients. Mentored participants in research.
- 2018. Mentorship Program for Aspiring Chemistry Teachers, University of Minnesota – Twin Cities.
    - Assisted in course planning and guest lecturing for an undergraduate quantum chemistry course.
- 2017. Student Teacher, Augsburg University, through Preparing Future Faculty, University of Minnesota – Twin Cities.
    - Prepared and delivered several lectures for a chemistry class for non-majors.
- 2014-2015. Teaching Assistant, University of Minnesota – Twin Cities, Chemistry Department. Honors General Chemistry lab, 44 to 48 students.
    - Led students in guided inquiry lab, graded all assignments.
    - Received the Robert L. Ferm Outstanding Graduate TA Award

PUBLICATIONS:

- Jeong, W. S.; **Stoneburner, S. J.**; King, D.; Li, R.; Walker, A.; Lindh, R.; Gagliardi, L. Automation of active space selection for multireference methods via machine learning on chemical bond dissociation. *J. Chem. Theory Comput.* **2020**, *16*, 2389–2399.
- **Stoneburner, S. J.;** Truhlar, D. G.; Gagliardi, L. Transition metal spin-state energetics by MC-PDFT with high local exchange. *J. Phys. Chem. A* **2020**, *124*, 1187–1195.
- Gaggioli, C. A.; **Stoneburner, S. J.**; Cramer, C. J.; Gagliardi, L. Beyond Density Functional Theory: the Multiconfigurational Approach to Model Heterogeneous Catalysis. *ACS Catal.*, **2019**, 9, 8481–8502.
- Demir, H.; **Stoneburner, S. J.**; Jeong, W.; Ray, D.; Zhang, X.; Farha, O. K.; Cramer, C. J.; Siepmann, J. I.; Gagliardi, L. Metal-Organic Frameworks with Metal Catecholates for O_2/N_2 Separation. *J. Phys. Chem. C* **2019**, *123*, 12935-12946.
- Presti, D.; **Stoneburner, S. J.;** Truhlar, D. G.; Gagliardi, L. Full Correlation in a Multiconfigurational Study of Bimetallic Clusters : Restricted Active Space Pair-Density Functional Theory Study of [2Fe-2S] Systems. *J. Phys. Chem. C* **2019**, *123*, 11899–11907.
- **Stoneburner, S. J.**; Gagliardi, L. Air Separation by Catechol-Ligated Transition Metals: A Quantum Chemical Screening. *J. Phys. Chem. C* **2018**, *122*, 22345–22351.
- **Stoneburner, S. J.**; Truhlar, D. G.; Gagliardi, L. MC-PDFT Can Calculate Singlet-Triplet Splittings of Organic Diradicals. *J. Chem. Phys.* **2018**, *148*, 064108.
- **Stoneburner, S. J.**; Shen, J.; Ajala, A. O.; Piecuch, P.; Truhlar, D. G.; Gagliardi, L. Systematic Design of Active Spaces for Multi-Reference Calculations of Singlet–Triplet Gaps of Organic Diradicals, with Benchmarks Against Doubly Electron-Attached Coupled-Cluster Data. *J. Chem. Phys.* **2017**, *147*, 164120.
- Ongari, D.; Tiana, D.; **Stoneburner, S. J.**; Gagliardi, L.; Smit, B. Origin of the Strong Interaction between Polar Molecules and Copper(II) Paddle-Wheels in Metal Organic Frameworks. *J. Phys. Chem. C* **2017**, *121*, 15135–15144.
- **Stoneburner, S. J.**; Livermore, V.; McGreal, M. E.; Yu, D.; Vogiatzis, K. D.; Snurr, R. Q.; Gagliardi, L. Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation. *J. Phys. Chem. C* **2017**, *121*, 10463–10469.
- Vogiatzis, K. D.; Li Manni, G.; **Stoneburner, S. J.**; Ma, D.; Gagliardi, L. Systematic Expansion of Active Spaces beyond the CASSCF Limit: A GASSCF/SplitGAS Benchmark Study. *J. Chem. Theory Comput.* **2015**, *11*, 3010–3021.
- Lee, K.; Isley, W. C.; Dzubak, A. L.; Verma, P.; **Stoneburner, S. J.**; Lin, L. C.; Howe, J. D.; Bloch, E. D.; Reed, D. A.; Hudson, M. R.; Brown, C. M.; Long, J. R.; Neaton, J. B.; Smit, B.; Cramer, C. J.; Truhlar, D. G.; Gagliardi, L. Design of a Metal-Organic Framework with Enhanced Back Bonding for Separation of N2 and CH4. *J. Am. Chem. Soc.* **2014**, *136*, 698–704.

PRESENTATIONS:

- *Affordable and Accurate Transition Metal Spin-State Energetics via MC-PDFT Using tPBE with High Local Exchange.*
    - 2019 Workshop on Recent Developments in Electronic Structure, University of Illinois – Urbana-Champaign, IL. May 2019. Poster
- *Computational Screening of Metal-Catecholate Functionalized Metal-Organic Frameworks for O_2/N_2 Separation*
    - Nanoporous Materials Genome Center all-hands meeting, University of Minnesota – Twin Cities, Minneapolis, MN. Sep. 2018. Oral and poster.
- *Air Separation by Metal-Catecholates in Metal-Organic Frameworks*
    - Dow Sustainability Innovation Student Challenge Award finalist presentations, University of Minnesota – Twin Cities, St Paul, MN. Dec. 2017. Oral and poster.
- *Air Separation with Metalated-Catecholates in Metal-Organic Frameworks*
    - Nanoporous Materials Genome Center all-hands meeting, University of Minnesota – Twin Cities, Minneapolis, MN. Oct. 2017. Oral and poster.
- *Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation*
    - Nanoporous Materials Genome Center all-hands meeting, University of Minnesota – Twin Cities, Minneapolis, MN. Oct. 2016. Oral and poster.
    - Junior/Senior Seminar, Hillsdale College, Hillsdale, MI. Sep. 2016. Invited talk.
    - Inorganometallic Catalyst Design Center all-hands meeting, University of Minnesota – Twin Cities, St. Paul, MN. Aug. 2016. Poster.
- *NO Binding to Catechol-Ligated Transition Metals: A CASPT2/DFT Study*
    - Nanoporous Materials Genome Center all-hands meeting, University of Minnesota – Twin Cities, St. Paul, MN. Oct. 2015. Poster.
    - Inorganometallic Catalyst Design Center all-hands meeting, University of Minnesota – Twin Cities, St. Paul, MN. Oct. 2015. Poster.
- *The Heart of Science: The Necessity of Liberal Motivations for Scientific Inquiry*
    - Honors program thesis defense, Hillsdale College, Hillsdale, MI. Apr. 2014. Oral.
- *Computational Study of Binding Properties for Methane/Nitrogen Separation Using Metal-Organic Frameworks*
    - MRSEC Summer Undergraduate Research Expo, University of Minnesota – Twin Cities, Minneapolis, MN. Aug. 2013. Poster.
    - Research program seminar, University of Minnesota – Minneapolis, MN. Jul. 2013. Oral.
- *Investigating Antibiotic Sorption on Model Soil Surfaces via Surface-Enhanced Raman Spectroscopy*
    - Hillsdale College Undergraduate Science Research Symposium, Hillsdale College, Hillsdale, MI. Mar. 2013. Poster
    - Junior/Senior Seminar, Hillsdale College, Hillsdale, MI. Oct. 2012. Oral.

RESEARCH:

- 2020–2022. Messiah University
    - Supervising undergraduate researchers calculating infrared spectra of polycyclic aromatic hydrocarbons.
- 2019–2021. Scientific Coordinator, Summer Undergraduate Research Fellowship in Computational and Theoretical Chemistry, University of Minnesota – Twin Cities.
    - Electronic structure calculations on catalytic cycles and molecular qubit candidates.
- 2014–2019. Research assistant. University of Minnesota – Twin Cities. Dr. Laura Gagliardi, advisor.
    - Development of multi-reference theory and application to gas separations.
- 2013. University of Minnesota – Twin Cities. Undergraduate researcher, LANDO program. Worked with Dr. Laura Gagliardi.
    - Used Gaussian and Molcas to calculate binding energies of small molecules with a metal-organic framework.
- 2012. Texas A&M University. Undergraduate researcher, NSF Research Experience for Undergraduates program. Worked with Dr. Dong Hee Son.
    - Synthesized quantum dots and studied them with NMR
- 2012. Hillsdale College. Undergraduate researcher, LAUREATES program. Worked with Dr. Matthew A. Young.
    - Used surface-enhanced Raman spectroscopy to analyze antibiotic sorption to model soil surfaces

SERVICE:

- 2021. Foster care provider in Cumberland County, Pennsylvania.
- 2017–2019. Foster care provider (leading to 4 adoptions) through Ramsey County, Minnesota.
- 2015–2019. Student contact for graduate recruitment at University of Minnesota.
- 2013–2014. American Chemical Society. Secretary of Hillsdale College chapter.

HONORS AND AWARDS:

- 2019. Overend Award in Physical Chemistry
- 2017. Finalist for Dow Sustainability Innovation Student Challenge Award
- 2016. Robert and Jill DeMaster Fellowship
- 2015. Robert L. Ferm Outstanding Graduate TA Award for general chemistry
- 2014. University of Minnesota – Twin Cities chemistry departmental fellowship

PROFESSIONAL AFFILIATIONS:

- 2010–Present. American Chemical Society. National Member.