Sara E. Mason
Department of Chemistry

Curriculum Vitae as of 04/14/22

Campus Address: W339 CB, University of Iowa
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EDUCATION AND PROFESSIONAL HISTORY

Post Graduate Education

2007 - 2010 **Postdoctoral Research Associate (National Research Council Fellow)**, Physics Laboratory, National Institute of Standards and Technology
Mentor(s): Dr. Anne M. Chaka (currently at PNNL)

Higher Education

May 2007 **Ph.D.**, Chemistry, University of Pennsylvania
Thesis: Quantum Mechanical Studies of Interactions in Model Catalytic Surfaces
Advisor: Prof. Andrew M. Rappe

May 2001 **B.S.**, Chemistry (Minor: Mathematics), *Summa cum laude*, St. John Fisher College
August 1999 **A.A.S.**, Chemical Technology, Monroe Community College

Professional and Academic Positions

2017-Present **Associate Professor**, Department of Chemistry, University of Iowa
2010-2017 **Assistant Professor**, Department of Chemistry, University of Iowa

Honors and Awards

2020 **Professional Development Award**, University of Iowa Office of the Executive Vice President and Provost
2020 **Emerging Investigator**, Environmental Science: Nano (*A Royal Society of Chemistry Journal*)
2014 **Rising Star Award**, St. John Fisher College Science Technology and Mathematics Alumni Association
2013 **NSF CAREER Award: Developing Quantum Nanogeochemistry for Molecular Studies and Inclusive Education**, Environmental Chemical Sciences Program
2012 **Emerging Investigator**, Journal of Environmental Monitoring
2007-2010 **NRC-NIST Research Associateship**, National Research Council

Memberships

2002-Present American Chemical Society
2003-Present American Physical Society
2008-Present Geochemical Society of America

SCHOLARSHIP

Publications

Refereed Journal Articles

2022:

54. Hudson, B. G., **Mason, S. E.** (**2022**). Metal Release and Electrical Properties of $Li_x(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$. *Applied Sciences, Accepted.*
53. Pyrch, M, M,, Augustine, L. J., Williams, J. A., **Mason, S. E.**, Forbes, T. Z. (**2022**). Use of Vibrational Spectroscopy to Identify the Formation of Neptunyl-Neptunyl Interactions: A Paired Density Functional Theory and Raman Spectroscopy Study. *Dalton Transactions, Accepted.*
52. Augustine, L. J., Abbaspour Tamijani, A., Bjorklund, J. L., Al-Abadleh, H. A., **Mason, S. E.** (**2022**). Adsorption of Small Organic Acids and Polyphenols on Hematite Surfaces: Density Functional Theory + Thermodynamics Analysis. *Journal of Colloid and Interface Science, 609* 469-481.
51. Abbaspour Tamijani, A., Augustine, L. J., Bjorklund, J. L., Catalano, J. G., **Mason, S. E.** (**2022**) First-Principles Characterization of Clean, Hydrated, and Defect α-Al_2O_3 and α-Fe_2O_3(110) Surfaces. *Molecular Simulation*, *48,* 247-263.

2021:

50. Henke, A. H., Ludadio, E. D., Hedlund, J. K., Abbaspour Tamijani, A., Hoang, K. N. L., **Mason, S. E.**, Murphy, C. J., Feng, Z. V., Hamers, R. J. (**2021**). Reciprocal Redox Interactions of Lithium Cobalt Oxide Nanoparticles with Nicotinamide Adenine Dinucleotide (NADH) and Glutathione (GSG): toward a Mechanistic Understanding of Nanoparticle-Biological Interactions. *Environmental Science: Nano, 8*, 1749-1760.
49. Metz, I. K., Bennett, J. W., **Mason, S. E.** (**2021**). Examining the Aufbau Principle and Ionization Energies: A Computational Chemistry Exercise for the Introductory Level. *Journal of Chemical Education, 98(12),* 4017-4025.
48. Bjorklund, J. L., Shohel, M., Bennett, J. W., Smith, J. A., Carolan, M., Hollar, E., Forbes, T. Z., **Mason, S. E.** (**2021**). Density Functional Theory and Thermodynamics Analysis of *M*Al_{12} Keggin Substitution Reactions: Insights into Ion Incorporation and Experimental Confirmation. *Journal of Chemical Physics, 154,* 064303 1-13.
47. Shohel, M., Bjorklund, J. L., Smith, J. A., Kravchuk, D. V., **Mason, S. E.**, Forbes, T. Z. (**2021**). Formation of nanoscale $[Ge_4O_{16}Al_{48}(OH)_{108}(H2O)_{24}]^{20+}$ from condensation of ε-$GeAl_{12}^{8+}$ Keggin polycations. *Angewandte Chemie, 60,* 8755-8759.
46. Alalwan, H. A., Augustine, L. J., Hudson, B. G., Abeysinghe, J. P., Gillan, E. G., **Mason, S. E.**, Grassian, V. H., Cwiertny, D. M. (**2021**). Linking Solid-State Reduction Mechanisms to Size-Dependent Reactivity of Metal Oxide Oxygen Carriers for Chemical Looping Combustion. *ACS Applied Energy Materials, 4(2),* 1163-1172.

2020:

45. Abbaspour Tamijani, A., Bjorklund, J. L., Augustine, L. J., Catalano, J. G., **Mason, S. E.** (**2020**). Density Functional Theory and Thermodynamics Modeling of Inner-Sphere Oxyanion Adsorption on the Hydroxylated α-Al_2O_3(001) Surface. *Langmuir, 36(44),* 13166-13180.
44. Ma, C., Borgatta, J., Hudson, B. G., Abbaspour Tamijani, A., De La Torre-Roche, R., Zuverza-Mena, N., Shen, Y, Elmer, W., Xing, B., **Mason, S. E.**, Hamers, R. J., White, J. C. (**2020**). Advanced material modulation of nutritional and phytohormone status alleviates damage from soybean sudden death syndrome. *Nature Nanotechnology, 15,* 1033-1042.
43. Shohel, M., Bjorklund, J. L., Ovrom, E., **Mason, S. E.**, Forbes, T. Z. (**2020**). Ga^{3+} incorporation into Al_{13} Keggin polyoxometalates and the formation of delta-$(GaAl11)^{7+}$ and $(Ga_{2.5}Al_{28.5})^{+19}$ polycations. *Inorganic Chemistry, 59(15),* 10461-1042.
42. Bennett, J. W., Jones, D. T., Hudson, B. G., Melendez-Rivera, J., Hamers, R. J., **Mason, S. E.** (**2020**). Emerging Investigator Series: First-Principles and Thermodynamics Comparison of Compositionally-Tuned Delafossites: Cation Release from the (001) Surface of Complex Metal Oxides *Environmental*

Science: Nano, 7, 1642-1651.

41. Pyrch, M., Bjorklund, J. L., Williams, J., Parr IV, D., **Mason, S. E.**, Leddy, J., Forbes, T. Z. (**2020**). Impacts of Hydrogen Bonding Interactions with $Np(V/VI)O_2Cl_4$ Complexes: Vibrational Spectroscopy, Redox Behavior, and Computational Analysis. *Dalton Transactions, 49,* 6854-6866.
40. Abbaspour Tamijani, A., Bennett, J. W., Jones, D. T., Carangena-Gonzalez, N., Jones, Z. R., Laudadio, E. D., Hamers, R. J., Santana, J. A., **Mason, S. E.** (**2020**). DFT and Thermodynamics Calculations of Surface Cation Release in $LiCoO^2$. *Applied Surface Science, 515,* 145865.
39. Hailu, A., Abbaspour Tamijani, A., **Mason, S. E.**, Shaw, S. K. (**2020**). Efficient Conversion of CO_2 to Formate Using Inexpensive and Easily Prepared Post-Transition Metal Alloy Catalysts. *ACS Energy & Fuels, 34(3),* 3467-3476.
38. Buchman, J. T., Bennett, E. A., Wang, C., Abbaspour Tamijani, A., Bennett, J. W., Hudson, B. G., Green, C. M., Clement, P. L., Zhi, B., Henke, A. H., Laudadio, E. D., **Mason, S. E.**, Hamers, R. J., Klaper, R. D., Haynes, C. L. (**2020**). Nickel Enrichment of Next-generation NMC Nanomaterials Alters Material Stability, Causing Unexpected Dissolution Behavior and Observed Toxicity to S. Oneidensis MR-1 and D. Magna. *Environmental Science: Nano, 7,* 571-587.

2019:

37. Bennett, J. W., Hudson, B. G., Metz, I. K., Liang, D., Spurgeon, S., Cui, Q., **Mason, S. E.** (**2019**). A systematic determination of Hubbard U using the GBRV ultrasoft pseudopotential set. *Computational Materials Science*, *170*, 109137-1--10.
36. Bjorklund, J. L., Pyrch, M. M., Basile, M. C., **Mason, S. E.**, Forbes, T. Z. (**2019**). Actinyl-cation interactions: Experimental and theoretical assessment of $[Np(VI)O_2Cl_4]^{2-}$ and $[U(VI)O_2Cl_4]^{2-}$ systems. *Dalton Transactions*, *48*, 8861-8871.
35. Bjorklund, J. L., Bennett, J. W., Forbes, T. Z., **Mason, S. E.** (**2019**). Modeling of MAl_{12} Keggin Heteroatom Reactivity by Anion Adsorption. *Cryst. Growth Des.*, *19*, 2820-2829.
34. Zhang, Y., Tamijani, A. A., Taylor, M. E., Zhi, B., Haynes, C. L., **Mason, S. E.**, Hamers, R. J. (**2019**). Molecular surface functionalization of carbon materials via radical-induced grafting of terminal alkenes. *Journal of the American Chemical Society*, *141*, 8277-8288.
33. Bennett, J. W., Raglione, M. E., Oburn, S. M., MacGillivray, L. R., Arnold, M. A., **Mason, S. E.** (**2019**). DFT Computed Dielectric Response and THz Spectra of Organic Co-Crystals and Their Constituent Components. *Molecules*, *24*, 959-986.
32. Bennett, J. W., Huang, X., Fang, Y., Cwiertny, D. M., Grassian, V. H., **Mason, S. E.** (**2019**). Methane dissociation on α-Fe_2O_3 (0001) and Fe_3O_4 (111) surfaces: First-principles insights into chemical looping combustion. *Journal of Physical Chemistry C*, *123*, 6450-6463.

2018:

31. Alalwan, H. A., **Mason, S. E.**, Grassian, V. H., Cwiertny, D. M. (**2018**). alpha-Fe_2O_3 Nanoparticles as Oxygen Carriers for Chemical Looping Combustion: An Integrated Materials Characterization Approach to Understanding Oxygen Carrier Performance, Reduction Mechanism, and Particle Size Effects. *Energy & Fuels*, *32*(7), 7959-7970.
30. Liang, D., Hong, J., Fang, D., Bennett, J. W., **Mason, S. E.**, Hamers, R. J., Cui, Q. (**2018**). Analysis of the conformational properties of amine ligands at the gold/water interface with QM, MM and QM/MM simulations. *Physical Chemistry Chemical Physics*, *20*, 3349-3362.
29. Bennett, J. W., Jones, D., Huang, X., Hamers, R. J., **Mason, S. E.** (**2018**). Dissolution of Complex Metal Oxides from First-Principles and Thermodynamics: Cation Removal from the (001) Surface of $Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$. *Environmental Science & Technology*, *52*(10), 5792-5802.
28. Bennett, J. W., Jones, D. T., Hamers, R. J., **Mason, S. E.** (**2018**). First-Principles and Thermodynamics Study of Compositionally Tuned Complex Metal Oxides: Cation Release from the (001) Surface of Mn-Rich Lithium Nickel Manganese Cobalt Oxide. *Inorganic Chemistry*, *57*(21), 13300-13311.
27. Bennett, J. W., Jones, D. T., Hamers, R. J., **Mason, S. E.** (**2018**). First-Principles and Thermodynamics Study of Compositionally Tuned Complex Metal Oxides: Cation Release from the (001) Surface of Mn-Rich Lithium Nickel Manganese Cobalt Oxide. *Inorganic Chemistry*, *57*, 13300-13311.

26. Laudadio, E. D., Bennett, J. W., Green, C. M., **Mason, S. E.**, Hamers, R. J. (**2018**). Impact of phosphate adsorption on complex cobalt oxide nanoparticle dispersibility in aqueous media. *Environmental Science & Technology*, *52*, 10186-10195.

25. Corum, K. W., Tamijani, A. A., **Mason, S. E.** (**2018**). Density functional theory study of arsenate adsorption onto alumina surfaces. *Minerals*, *8*.

2017:

24. Bennett, J. W., Bjorklund, J. L., Forbes, T. Z., **Mason, S. E.** (**2017**). Systematic Study of Aluminum Nanoclusters and Anion Adsorbates. *Inorganic Chemistry*, *56*, 13014–13028.

23. Huang, X., Bennett, J. W., Hang, M. H., Laudadio, E., Hamers, R. J., **Mason, S. E.** (**2017**). Ab Initio Atomistic Thermodynamics Study of the (001) Surface of $LiCoO_2$ in a Water Environment and Implications for Reactivity under Ambient Conditions. *Journal of Physical Chemistry C*, *121*, 5069-5080.

22. Gunsolus, I. L., Hang, M. N., Hudson-Smith, N. V., Buchman, J. T., Bennett, J. W., Conroy, D., **Mason, S. E.**, Hamers, R. J., Haynes, C. L. (**2017**). Influence of Nickel Manganese Cobalt Oxide Nanoparticle Composition on Toxicity Toward Shewanella One. *Environmental Science: Nano*, *4*, 636-646.

21. Corum, K., Huang, X., Bennett, J., **Mason, S. E. (2017**). Systematic Density Functional Theory Study of the Structural and Electronic Properties of Constrained and Fully Relaxed (001) Surfaces of Alumina and Hematite. *Molecular Simulation*, *43*(5-6), 406-419.

2016 And Earlier:

20. Huang, X., Ramadugu, S. K., **Mason, S. E. (2016**). Surface-Specific DFT + *U* Approach Applied to α-Fe2O3(0001). *Journal of Physical Chemistry C*, *120*, 4919-4930.

19. Cui, Q., Hernandez, R., **Mason, S. E.**, Frauenheim, T., Pedersen, J., Geiger, F. (**2016**). Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. *Journal of Physical Chemistry B*, *120*, 7297–7306.

18. Corum, K. W., **Mason, S. E.** (**2016**). Using density functional theory to study shape-reactivity relationships in Keggin Al-nanoclusters. *Water Research*, *102*, 413-420.

17. Corum, K. W., Fairley, M., Unruh, D. K., Payne, M. K., Forbes, T. Z., **Mason, S. E.** (**2015**). Characterization of Phosphate and Arsenate Adsorption onto Keggin-Type Al_{30} Cations by Experimental and Theoretical Methods. *Inorganic Chemistry*, *54*(17), 8367-8374.

16. Ramadugu, S. K., **Mason, S. E.** (**2015**). DFT Study of Antimony(V) Oxyanion Adsorption on α-Al2O3(1$\bar{1}$02). *Journal of Physical Chemistry C*, *119*(32), 18149-18159.

15. Fairley, M., Corum, K. W., Johns, A., Unruh, D. K., Basile, M., de Groot, J., **Mason, S. E.**, Forbes, T. Z. (**2015**). Isolation and characterization of the $[Ga_2Al_{18}O_8(OH)_{36}(H_2O)_{12}]^{8+}$ cluster: cationic variations on the Wells–Dawson topology. *Chemical Communications*, *51*(62), 12467-12469.

14. Huang, X., **Mason, S. E.** (**2014**). DFT-GGA Errors in NO Chemisorption Energies on (111) Transition Metal Surfaces. *Surface Science*, *621*, 23-30.

13. **Mason, S. E.**, Corum, K. W., Ramadugu, S. K. **(2014**). Fundamental Insights about Environmental Interface Reactivity from DFT Calculations of Geochemical Model Systems. *Surface Science*, *631*, 48-56.

12. Corum, K. W., **Mason, S. E.** (**2014**). Establishing Trends in Ion Adsorption on the Aqueous Aluminum Hydroxide Nanoparticle Al30. *Molecular Simulation*, *41*(1-3), 146-155.

11. Abeysinghe, S., Corum, K. W., Neff, D. L., **Mason, S. E.**, Forbes, T. Z. (**2013**). Contaminant Adsorption on Nanoscale Particles: Structural and Theoretical Characterization of Cu2+ Bonded to the Surface of Keggin-Type Polyaluminum (Al_{30}) Species. *Langmuir*, *29*(46), 14124-14134.

10. Goffinet, C. J., **Mason, S. E.** (**2012**). Comparative DFT Studies of Inner-Sphere As(III) Complexes on Hydrated α-Fe_2O_3(0001) Surface Models. *Journal of Environmental Monitoring*, *14*(7), 1860-1871.

9. **Mason, S. E.**, Trainor, T. P., Goffinet, C. J. (**2012**). DFT Study of Sb(III) and Sb(V) Adsorption and Heterogeneous Oxidation of Hydrated Oxide Surfaces. *Computational and Theoretical Chemistry*, *987*, 103-114.

8. **Mason, S. E.**, Trainor, T. P., Chaka, A. M. (**2011**). Hybridization-Reactivity Relationship in Pb(II)

Adsorption on α-Al_2O_3-Water Interfaces: A DFT Study. *Journal of Physical Chemistry C*, *115*(10), 4008-4021.

7. **Mason, S. E.**, Iceman, C. R., Trainor, T. P., Chaka, A. M. (**2010**). Molecular-Level Understanding of Environmental Interfaces Using Density Functional Theory Modeling. *Physics Procedia*, *4*, 67-83
6. **Mason, S. E.**, Iceman, C. R., Trainor, T. P., Chaka, A. M. (**2010**). Density Functional Theory Study of Clean, Hydrated, and Defective Alumina (1-102) Surfaces. *Physical Review B*, *81*(12543), 1-16.
5. **Mason, S. E.**, Sokol, E. A., Cooper, V. R., Rappe, A. M. (**2009**). Spontaneous formation of dipolar metal nanoclusters. *J. Phys. Chem. A*, *113*, 4134--37.
4. **Mason, S. E.**, Grinberg, I., Rappe, A. M. **(2008**). Orbital-specific analysis of CO chemisorption on transition-metal surfaces. *J. Phys. Chem. C*, *112*, 1963--66.
3. Grinberg, I., Suchomol, M. R., Dmowski, W., **Mason, S. E.**, Wu, H., Davies, P. J., Rappe, A. M. (**2007**). Structure and Polarization in the High T_c Ferroelectric Bi(Zn,Ti)O_3-$PbTiO_3$ Solid Solutions. *Phys. Rev. Lett.*, *98*, 107601:1-4.
2. **Mason, S. E.**, Grinberg, I., Rappe, A. M. (**2006**). Adsorbate-adsorbate interactions and chemisorption at different coverages studied by accurate ab initio calculations: CO on transition metal surfaces. *J. Phys. Chem. B*, *110*, 3816--22.
1. **Mason, S. E.**, Grinberg, I., Rappe, A. M. (**2004**). First-principles extrapolation method for accurate CO adsorption energies on metal surfaces. *Phys. Rev. B*, *69*, 161401R-1--4.

Non-refereed Articles

1. (2017). Research highlights: comparing the biological response of nanoparticle solid solutions. *Environmental Science Nano*, *4*, 1428-1432.

Book Chapters

1. Mason, S. E. (2018). On Our Own Terms. K. Woznack, A. Charlebois, R. Cole, C. Marzabadi, & G. Webster (Eds.), *Mom the Chemistry Professor: Personal Accounts from Chemistry Professors who are Mothers, 2nd Edition*. Springer. https://www.springer.com/la/book/9783319789712

Education Guide

1. Mason, S. E., as part of a 13 member taskforce: *Chemistry Transition Guide 2014: A production coordinated by the Governor's STEM Advisory Council Administration Office.* https://iowastem.org/sites/default/files/transition-guides/chemistryguide-revised-final_1-6-14_1.pdf

Theses and Dissertations

1. Judy He. *Density Functional Theory Modeling of Geochemical Model Systems to Elucidate Differences in Aluminum Oxide Surface and Nanoparticle Reactivity.* Undergraduate Honors Thesis, University of Iowa, 2014.
2. Katie Corum (Witkin). *Theoretical Discovery of Shape-Reactivity Relationships in Aluminum Nanoclusters*. Ph.D. University of Iowa, 2016.
3. Xu Huang. *Extending Accurate Density Functional Modeling for the Study of Interface Reactivity and Environmental Applications.* Ph.D. University of Iowa, 2017.
4. Jennifer L. Bjorklund. *First-Principles Insights on Aluminum Nanocluster Reactivity and Crystallization for Environmental Remediation.* Ph.D. University of Iowa, 2020.
5. Irene K. Metz. *From First-Year Chemistry to Materials Design: The Versatility of Computational Chemistry.* Ph.D. University of Iowa, 2021.
6. Diamond T. Jones. *Frist Principles and Thermodynamics Approach to Understanding Metal Release from Complex Metal Oxides.* Ph.D. University of Iowa, 2021

Articles Under Review

Liang, D., Liu, J., Heinz, H., **Mason, S. E.**, Hamers, R. J., and Cui, Q. Binding of Polar and Hydrophobic Molecules at the $LiCoO_2$(001)-water Interface: Force Field Development and Molecular Dynamics Simulations. *Nanoscale, Submitted 2/4/2022, Decision of "Major Revisions" as of 3/25/2022.*

Areas of Research Interest

Physical chemistry, computational chemistry, electronic structure calculations, density functional theory, thermodynamics modeling, molecular dynamics, complex metal oxides, nanomaterials, nanoclusters, surfaces, mineral-water interfaces, adsorption, surface processes, transformations.

I established my research group at the University of Iowa in 2010, with the goal of using theory and modeling to develop molecular-level understanding of *environmental interfaces*. Environmental interfaces refer to surfaces (including the exposed surfaces of nanophases) in equilibrium with their surroundings. The chemically motivated problems probed by research in my group include: Why do some mineral surfaces form strong bonds to aqueous contaminants, while others do not? How does the shape of aqueous metal hydroxide clusters relate to properties and reactivity? How does exposure to the environment transform the structure and chemistry of technologically relevant nanomaterials? The primary research tool in my group is density functional theory (DFT), a robust quantum mechanical framework for the atomic modeling of molecular systems, bulk materials, and interfaces. To take DFT out of the vacuum, we use the outputs of DFT calculations as inputs in models that go on to incorporate statistical mechanics, electrochemical principles, and thermochemical data. The resulting DFT + Thermodynamics methodologies are robust and adaptable to the study of a wide range of chemical processes occurring at environmental interfaces and allows theory and modeling to bridge macroscopic behavior to molecular-level understanding.

Funded/Awarded Grants and Contracts

Sep 2020 – Aug 2025	*The NSF Center for Sustainable Nanotechnology* Funded by NSF-CHE-CCI PI is Robert J. Hamers, University of Wisconsin-Madison. Mason is Senior Personnel Full Award Amount: $20,000,000.00. Annual UI subcontract (Mason) ~$170,000.
Sep 2020 – Aug 2024	*NSF RII Track-2 FEC: Data-enabled Discovery and Design to Transform Liquid-based Energy Storage (D3TaLES)* Funded by NSF-OIA PI is Chad Risko, University of Kentucky. Mason is a co-PI. Full award is $3,979,525. Annual UI subcontract (shared with Shaw) ~$140,000.
Sep 2015 - Aug 2020	*Phase II Center for Chemical Innovation, A Molecular Basis for Sustainable Nanotechnology* Funded by NSF-CHE-CCI. Award amount: ($20,000,000.00). Mason is Senior Personnel. The final amount for the UI subcontract was: $759,305.

Sep 2015 – Aug 2018	*Collaborative Research: Interfacial Water Restructuring: An Unrecognized Contribution to Mineral Surface Reactivity* Funded by NSF-CHE-ECS. Award amount: ($240,000.00). Collaborator: Prof. Jeffrey G. Catalano, Department of Earth and Planetary Science, Washington University in St. Louis.
Sept 2015 – Aug 2018	*Insights into Chemical Looping Combustion Through a Combined Theory and Experimental Approach* Funded by NSF-ENG-CBET. Award amount: ($299,878.00).
Jun 2013 – May 2018	*CAREER: Developing Quantum Nanogeochemistry for Molecular Studies and Inclusive Education* Funded by NSF-CHE-ECS. Award amount: ($525,000.00).
Aug 2013 - Jul 2014	*Theoretical Description of Nanomaterials for Water Remediation* Funded by Center for Global & Regional Environmental Research Seed Grant Program. Award amount: ($30,000.00).
Jul 2012 – Jun 2013	*Theoretical Discovery of Universal Reactivity Factors Describing Environmental Interfaces* Funded by Mathematical and Physical Sciences Funding Program. Award amount: ($25,000.00).
Awarded Computer Time Grants	
Oct 2021- Sept 2022	*Density Functional Theory Calculations for Nanomaterials in Energy Applications and the Environment* Funded by NSF-XSEDE. Investigator/s Sara E Mason (Principal Investigator), Logan J. Augustine (Co-Principle).
Oct 2020 – Sept 2021	*Density Functional Theory Calculations for Nanomaterials in Energy Applications and the Environment* Funded by NSF-XSEDE. Investigator/s Sara E Mason (Principal Investigator), Ali Abbaspour Tamijani (Co-Principal).
Oct 2017 - Sep 2018	*Density Functional Theory Calculations for Nanomaterials in Energy Applications and the Environment* Funded by NSF-XSEDE. Investigator/s Sara E Mason (Principal Investigator), Joseph W Bennett (Co-Principal)
Oct 2016 - Sep 2017	*Density Functional Theory Calculations for Nanomaterials in Energy Applications and the Environment* Funded by NSF-XSEDE. Investigator Sara E Mason
Oct 2014 - Sep 2015	*Project UAFAQUA: Structure and Reactivity of Aqueous Geochemical Interfaces* Funded by Artic Region Super Computing Center, University of Alaska Fairbanks.
Oct 2013 - Sep 2014	*Project UAFAQUA: Structure and Reactivity of Aqueous Geochemical Interfaces* Funded by Arctic Region Super Computing Center, University of Alaska

	Fairbanks.
Oct 2012 - Sep 2013	*Project UAFAQUA: Structure and Reactivity of Aqueous Geochemical Interfaces* *Arctic Region Super Computing Center, University of Alaska Fairbanks*

Internal

PROGRAM	ROLE	AMOUNT	YEAR
Center for Global and Regional Environmental Research Seed Grant Program	PI	$30,000	Aug 2013-Jul 2013
Mathematical and Physical Sciences Funding Program	PI	$25,000	Jul 2012-Jun 2013

Invited Lectures and Conference Presentations

International Conferences

2021	*AVS 67th International Symposium and Exhibition* *"Designed Metal Release from Complex Metal Oxides"* *Charlotte North Carolina, United States* *Presenters/Authors:* ***Mason****, Sara E.*
2020 (delayed, ultimately cancelled)	*The International Chemical Congress of Pacific Basin Societies (Pacifichem)* *"Modeling Complex Metal Oxide Structure and Transformations in Aqueous Media,"* *Honolulu, Hawaii, United States* *Presenters/Authors:* ***Mason****, Sara E.*
2019	*AVS 66th International Symposium and Exhibition* *"Theoretical Modeling of Metal Release from Complex Metal Oxides," Columbus, Ohio, United Sates* *Presenters/Authors:* ***Mason****, Sara E.*
2018	*13th International Conference on the Environmental Effects of Nanoparticles and Nanomaterials,* *"Modeling Dissolution of Complex Metal Oxides from First-Principles and Thermodynamics," Duke University, Durham North Carolina, United States* *Presenters/Authors:* ***Mason****, Sara E.*
2017	*Centre Europeen de Calcul Atomique et Moleceulaire (CECAM) Tackling Complexity of the Nano-Bio Interfaces,* *"DFT Methods for Solid-Liquid Interfaces," Bremen University, Bremen, German* *Presenter/Authors: Bennett, Joseph W. and* ***Mason****, Sara E. (Bennett spoke as Mason was medically unable to travel.)*
2016	*Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, "Theoretical Discovery of Reactivity Factors in Al Nanocluster Adsorption," Center for Simulational Physics, Athens, Georgia, United States* *Presenters/Authors:* ***Mason****, Sara E*

National Conferences

2022	*American Chemical Society, Quantum Chemistry on the Computer: The Terminal is a Window to a New World, San Diego, California*
2021	*American Chemical Society, Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Surface Processes in Aqueous Environments, Virtual. Presenters/Authors: **Mason**, Sara E.*
2021	*American Chemical Society, Resilience of Women in Chemistry, Webinar/Virtual. Presenters/Authors: **Mason**, Sara E.*
2018	*Biennial Conference on Chemical Education, On Our Own Terms: Mom the Chemistry Professor, South Bend, Indiana Presenters/Authors: **Mason**, Sara E.*
2016	*American Chemical Society, First-Principles Discovery of Shape-Reactivity Relationships in Adsorption onto Keggin-Type Aluminum Hydroxides, Philadelphia, Pennsylvania, United States. Presenters/Authors: **Mason**, Sara E*
2012	*American Chemical Society, DFT Studies of Arsenate and Arsenite Surface Complexes on Ideal and Defective Hematite-Water Interfaces, San Diego, California, United States Presenters/Authors: **Mason**, Sara E*

Regional Conferences

2021	*AVS Prairie Chapter, Designed Metal Release in Aqueous Media from Complex Metal Oxides, Virtual. Presenters/Authors: **Mason,** Sara E.*
2019	*Midwest Theoretical Chemistry Conference, Building bridges between computational chemistry and experiment at the nanoscale: Impacts on energy and the environment, South Bend, Indiana Presenters/Authors: **Mason**, Sara E*
2018	*2018 Midwest Regional Meeting of the American Chemical Society, Modeling Nanomaterial Reactivity, Transformations, and Dissolution through Electronic Structure Calculations, Thermodynamics, and Electrochemical Principles, Ames, Iowa Presenters/Authors: **Mason**, Sara E*

Keynote/Plenary Address

2019	Third Annual Research Symposium, *Computational Chemistry of Nanomaterials in Energy & the Environment*, University of Peurto Rico RISE Program, Cayey, Puerto Rico Presenters/Authors: Mason, Sara E.

Regional

2018	Midwest Women Chemists Retreat, *DFT Investigation of Aluminum Nanocluster Reactivity*, Decorah Presenters/Authors: Mason, Sara E Student Presenters/Authors: Bjorklund, Jennifer L

Invited Seminars at External Departments (Mason is author/presenter in all, unless otherwise noted)

2022 *Predicting the Thermodynamics of Aqueous Adsorption at Mineral Surfaces*. Environmental Thermochemistry Research Group, Georgia State University. Presenter/Author: Mason, Sara E.

2022 *Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Impacts on Energy, Agriculture, and the Environment.* NASA-MIRO: Center for Advanced Manufacturing in Space & Technology Research at University of District of Columbia. Presenter/Author: Mason, Sara E.

2022 *Electronic Structure and Thermodynamics Modeling of Nanomaterial Transformations.* Seminar, Center for Functional Nanomaterials, Brookhaven National Lab. Presenter/Author: Mason, Sara E.

2022 *Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Impacts on Energy, Agriculture, and the Environment.* Chemistry Seminar, George Mason University. Presenter/Author: Mason, Sara E.

2021 *Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Impacts on Energy, Agriculture, and the Environment.* Chemistry Seminar, University of Maryland. Presenter/Author: Mason, Sara E.

2021 *Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Impacts on Energy, Agriculture, and the Environment.* Chemistry Seminar, Washington University at St. Louis. Presenter/Author: Mason, Sara E.

2021 *Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Impacts on Energy and the Environment.* Physical Chemistry Seminar, University of Illinois Urbana-Champaign. Presenter/Author: Mason, Sara E.

2021 *Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Impacts on Energy, and the Environment,* Department of Chemistry, Bradley University, Peoria, Illinois Presenter/Author: Mason, Sara E. (Recruiting talk.)

2021 *Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Impacts on Energy, and the Environment*, Department of Chemistry, Truman State University, Missouri Presenter/Author: Mason, Sara E. (Invited by Student ACS Chapter.)

2019 *Designed Metal Release from Complex Metal Oxides*, Physical Chemistry Seminar, University of Pennsylvania, Philadelphia Presenters/Authors: Mason, Sara E

2019 *Building Bridges between Computational Chemistry and Experiment at the Nanoscale: Impacts on Human Health, Energy, and the Environment*, Department of Chemistry, Dartmouth College, Hanover, New Hampshire, United States Presenters/Authors: Mason, Sara E

2018 *Modeling Cation Release from Compositionally Tuned Complex Metal Oxides from First Principles*, Materials Chemistry Seminar Series, University of Wisconsin Madison, Madison, Wisconsin Presenters/Authors: Mason, Sara E

2018 *Computational Chemistry to Understand Nanomaterials in the Environment*, Drake University, Des Moines, Iowa Presenters/Authors: Mason, Sara E

2017 *Molecular-level insights into the biological impact of Li battery materials from DFT and thermodynamics modeling*, University of California San Diego

2016 *Fundamental Insights about Aluminum Nanoclusters and Mineral Surfaces from Density Functional Theory*, Oregon State University, Corvallis, Oregon, United States Presenters/Authors: Mason, Sara E

2016 *Fundamental Insights about Aluminum Nanoclusters and Mineral Surfaces from Density Functional Theory*, University of Oregon, Joint Materials Science Institute and Physical Chemistry Seminar, Eugene, Oregon, United States Presenters/Authors: Mason, Sara E

2016 *Theoretical Discovery of Reactivity Factors in Al Nanocluster Adsorption*, Materials Theory Group, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States Presenters/Authors: Mason, Sara E

2016 *"Fundamental Insights about Geochemical Surface Science from Density Functional Theory"*, Washington University Dept. of Earth and Planetary Science, St. Louis, Missouri, United States Presenters/Authors: Mason, Sara E

2015 *"Environmental Geochemistry from First Principles"*, William Jewell College, Department of Chemistry, Liberty, Iowa, United States Presenters/Authors: Mason, Sara E This was a recruiting talk at a primarily undergraduate institution.

2015 *"Fundamental Insights about Geochemical Surface Science from Density Functional Theory"*, University of Minnesota, Department of Chemistry, Minneapolis, Minnesota, United States Presenters/Authors: Mason, Sara E

2015 *"Fundamental Insights from DFT Calculations of Geochemical Model Systems"*, Michigan State University, Department of Chemistry, Lansing, Michigan, United States Presenters/Authors: Mason, Sara E

2015 *"Fundamental Insights from DFT Calculations of Geochemical Model Systems"*, Penn State University, Department of Chemistry, College Park, Pennsylvania, United States Presenters/Authors: Mason, Sara E

2015 *"Fundamental Insights from DFT Calculations of Geochemical Model Systems" U*, University of Missouri, Department of Chemistry, Columbia, Missouri, United States Presenters/Authors: Mason, Sara E

2015 *"Fundamental Insights from DFT Calculations of Geochemical Model Systems"*, Wayne State University Department of Chemistry, Detroit, Michigan, United States Presenters/Authors: Mason, Sara E

2015 *Fundamental Insights from DFT Calculations of Geochemical Model Systems*, St. Cloud State University, Department of Chemistry

2015 *Fundamental Insights from DFT Calculations of Geochemical Model Systems*, The Ohio State University, Department of Chemistry

2014 *Molecular-Level Understanding of Aqueous Aluminum Hydroxide Nanoparticle Reactivity through DFT Studies*, Grinnell College Department of Chemistry

2013 *Environmental Geochemistry from First Principles*, Knox College, Department of Chemistry, Galesburg, Illinois, United States

2013 *Improving Drinking Water One Ion at a Time!*, Coe College, Department of Chemistry, Cedar Rapids, Iowa. Presenters/Authors: Corum, Katie W, Mason, Sara E

2013 Department of Materials Science and Engineering, *Exploring Bonding Competition and Adsorption-Induced Substrate Changes through DFT Calculations of Geochemical Models*, Iowa State University, Ames, Iowa, United States

Talks at University of Iowa

2022 University of Iowa Department of Physics, Condensed Matter Division, *Metal Release from Complex Metal Oxides by Design: Modeled using Electronic Structure Calculations and Thermodynamics Modeling*, University of Iowa, Iowa City

2020 University of Iowa Interdisciplinary Graduate Program in Applied Mathematics and Computational Sciences, *From the Atomic Scale to Biological Impact: Ab initio Thermodynamics Modeling of Nanomaterials in the Environment,* University of Iowa, Iowa City
Presenters/Authors: Mason, Sara E

2018 University of Iowa Nanoscience and Nanotechnology Institute, *Combining Electronic Structure Calculations and Thermodynamics Modeling to Predict Nanomaterial Reactivity, Transformation, and Dissolution*, University of Iowa, Iowa City

2018 Presenters/Authors: Mason, Sara E.
University of Iowa Showcase on Sustainability, *Computational Chemistry of*
2012 *Sustainable Nanotechnology,* University of Iowa, Iowa City
Presenters/Authors: Mason, Sara E.
University of Iowa Water Sustainability Initiative, *Theoretical Insights about the Reactive Properties of Hydrated Surfaces*, University of Iowa, Iowa City
Presenters/Authors: Mason, Sara E.

Contributed Conference Presentations

National Conferences

2018 ACS National Meeting, *Aluminum Hydroxide Nanocluster Reactivity Studied Through Computational Chemistry,* New Orleans, Louisiana, United States.
2017 ACS National Meeting, *Theoretical Studies of Prenucleation Clusters,* Washington, District of Columbia, United States.
2013 ACS National Meeting, *Predicting Aqueous Aluminum Hydroxide Nanoparticle Reactivity*, New Orleans, Louisiana, United States.
2012 ACS National Meeting, *Theoretical Studies of the Reactive Properties of Environmental Oxide Nanomaterials*, San Diego, California, United States

Regional Conferences

2013 Midwest Theoretical Chemistry Conference, *Identifying and Correcting for DFT-GGA Errors in NO Chemisorption Energies on Transition Metal Surfaces*, Champaign, Illinois, United States Presenters/Authors: Hang, Xu, Mason, Sara E
2013 Midwest Theoretical Chemistry Conference, *Reactivity Between Aqueous Cu(II) and Aluminum Hydroxide Nanoparticles: New Mechanistic Insights from DFT-Based Simulations*, Champaign, Illinois, United States Presenters/Authors: Corum, Katie W, Mason, Sara E

Student Conference Presentations

National Conferences

2022 ACS National Meeting, *First Principles and Thermodynamics Modeling of Ti_3C_2T3 MXene Surface Terminations at Varying pH*, San Diego, California, United States. Presenters/Authors: Rivera, Victoria M., Mason, Sara E.
2022 ACS National Meeting, *Training a Machine Learning Model to Predict Metal Release from Complex Metal Oxide Surfaces*, San Diego, California, United Sates. Presenters/Authors: Hudson, Blake G., Mason, Sara E.
2022 ACS National Meeting, *A Computationally-Guided Assignment of the Vibrational Features of Neptunyl Engaged in Actinyl-Actinyl Interactions,* San Diego, California, United States. Presenters/Authors: Augustine, Logan J., Pyrch, Mikaela, Forbes, Tori Z., Mason, Sara E.
2021 ACS National Meeting, *Modeling surface and media dependent facets of Cu from nano agriculture materials,* Virtual. Presenters/Authors: Hudson, Blake G, Mason, Sara E.
2021 ACS National Meeting, *A DFT + Thermodynamics Model of Study Inner-sphere*

Adsorption Occurring at the Mineral-Water Interface, Virtual. Presenters/Authors: Augustine, Logan J., Borklund, Jennifer L., Abbaspour Tamijani, A., Mason, Sara E.

2019 ACS National Meeting, *Using DFT, molecular dynamics, and thermodynamics modelling, to connect with experimental information about Al_2O_3-water interface structure and reactivity*, Orlando, Florida Presenters/Authors: Mason, Sara E, Tamijani, Ali A

2019 ACS National Meeting, *DFT + Thermodynamics Prediction of MAl12 Keggin Heteroatom Reactivity and Substitution*, Orlando, Florida, United States Presenters/Authors: Bjorklund, Jennifer L, Mason, Sara E

2018 ACS National Meeting, *Systematic Determination of Hubbard U for High-Throughput DFT Calculations,* New Orleans, Louisiana, United States Presenters/Authors: Spurgeon, Sidney, Bennett, Joseph, Metz, Irene, Hudson, Blake, Mason, Sara E.

2018 Biennial Conference on Chemical Education, *Computational Chemistry in Community College Education and Research*, South Bend, Indiana, United States Presenters/Authors: Metz, Irene K, Mason, Sara E.

2018 Biennial Conference on Chemical Education, *Materials Design in the Community College: A First-Principles Approach to Band Gap Tuning, South Bend*, Indiana, United States Presenters/Authors: Metz, Irene K, Mason, Sara E.

2014 American Physical Society Meeting, *Density Functional Theory Studies of Sb(V) Oxyanion Adsorption on α-Al_2O_3 Surfaces*, Denver, Colorado, United States Presenters/Authors: Ramadugu, Sai Kumar, Mason, Sara E.

2014 American Physical Society Meeting, *Surface-Specific Hubbard U Calculations for α-Fe_2O_3(0001) Surfaces*, Denver, Colorado, United States Presenters/Authors: Huang, Xu, Ramadugu, Sai Kumar

2013 ACS National Meeting, *DFT Studies of Sb(V) Adsorption on α-Al_2O_3 and α-Fe_2O_3*, Indianapolis, Indiana, United States Presenters/Authors: Ramadugu, Sai K, Mason, Sara E

2013 ACS National Meeting, *Extending Computational Research Opportunities to Multidisciplinary University Students*, Indianapolis, Indiana, United States

2013 ACS National Meeting, *Modeling the Uptake of Oxyanion and Cation Contaminant Species by Aqueous Aluminum Hydroxide Nanoparticles*, Indianapolis, Indiana, United States Presenters/Authors: Corum, Katie W, Forbes, Tori Z, Mason, Sara E

Regional Conferences

2019 1st American-Mexican Symposium on Supramolecular Materials Design, *First Principles Modeling of Lithium Intercalation Materials*, Iowa City, Iowa, United States. Presenters/Authors: Hudson, Blake G., Jones, Diamond T., Melendez, Joshua., Hamers, Robert J., Mason, Sara E.

2018 Midwest Theoretical Chemistry Conference, *Thermodynamics of Complex Metal Oxide Transformations,* Chicago, Illinois, United States. Presenters/Authors: Bennett, Joseph W., Mason, Sara E.

Posters

2022 ACS National Meeting, *Adsorption of Organic Redox-Active Molecules on the Ag(111) Surface,* San Diego, California, United States. Presenters/Authors: Sweet, Amelia and Mason, Sara E.

2022	ACS National Meeting, *A Mechanistic Study of Secondary Cation Release from the (001) Surface of Li($Ni_yMn_zCo_{1-y-z}$)O_2,* San Diego, California, United States. Presenters/Authors: Jones, Diamond T., Hudson, Blake G., Rivera, Victoria M, Bennett, Joseph W., Mason, Sara E.
2021	ACS National Meeting, *Systematic Study of the Effect of Inner-Sphere Adsorption of Alkali Metals and Alkaline Earth Anions on the (101) alpha-Quartz Surface on Dissolution Energetics*, Virtual. Presenter/Authors: Jones, Diamond T., Mason, Sara E.
2021	ACS National Meeting, *A Hands-On Approach to the Aufbau Principle through Computational Chemistry,* Virtual. Presenter/Authors: Metz, Irene K., Mason, Sara E.
2019	The 31st Annual Workshop on Recent Developments in Electronic Structure Methods, *A High-Throughput Approach to DFT + U*, Urbana-Champaign, Illinois. Presenters/Authors: Mason, Sara E, Bennett, Joseph W Student Presenters/Authors: Hudson, Blake G, Jones, Diamond T
2019	The 31st Annual Workshop on Recent Developments in Electronic Structure Methods, *Designed Metal Release From Complex Metal Oxides*, Urbana-Champaign, Illinois Presenters/Authors: Mason, Sara E, Tamijani, Ali A, Bennett, Joseph W Student Presenters/Authors: Jones, Diamond T, Hudson, Blake G
2018	Midwest Theoretical Chemistry Conference, *Systematic Determination of Hubbard U for High-Throughput DFT Calculations*, Chicago, Illinois, United States. Presenters/Authors: Hudson, Blake G., Bennett, Joseph W., Mason, Sara E.
2013	ACS National Meeting, *Identifying and Correcting For DFT-GGA Errors in NO Chemisorption Energies on Transition Metal Surfaces*, Indianapolis, Indiana, United States Presenters/Authors: Hang, Xu, Mason, Sara E
2013	ACS National Meeting, *DFT Studies of how Particle History and Bonding Competition Affect Reactivity in Model Rutile TiO2-Water Interfaces*, New Orleans, Louisiana, United States Presenters/Authors: Mason, Sara E

SERVICE

Profession

2022	National Science Foundation Panel Reviewer
2021	Department of Energy Ad Hoc Proposal Reviewer
2021	Advisory Board: Environmental Science:Nano *A Royal Society of Chemistry journal*
2021	MolSSI Computational Chemistry Workshop for Undergraduates: Delivered overview talk on Quantum Chemical Methods. The Molecular Sciences Software Institute (MolSSI) is NSF funded, and this was an outreach/education activity held at the Tapia Center for Equity and Excellence at Rice University.
2021	Speaker and Panelist, American Chemical Society Women Chemists Committee Webinar on "Resilience of Women in Chemistry."
2021	National Science Foundation Panel Reviewer
2020-Present	Executive Committee, NSF for Sustainable Nanotechnology (manage a portfolio of projects, review bi-monthly reports of ~70 trainees, provide steering guidance on center research directions)
2020	American Chemical Society, ACS Award for Computers in Chemical and Pharmaceutical

	Research, Committee Assignment
2020	National Science Foundation Panel Reviewer, Two Panels
2020	Reviewed 5 journal manuscripts
2019	Reviewed 4 journal manuscripts
2019	American Chemical Society, ACS Award for Computers in Chemical and Pharmaceutical Research, Committee Assignment
2019	National Science Foundation Panel Reviewer
2018	Diversity Committee, NSF Center for Sustainable Nanotechnology
2018	Reviewed 5 journal manuscripts
2018	National Science Foundation Panel Reviewer, Two Panels
2017	Reviewed 5 journal manuscripts
2016	Reviewed 7 journal manuscripts
2016	Participant in the NSF Workshop on Midscale Instrumentation: Regional Facilities to Address Grand Challenges in Chemistry, held in Arlington VA September 29-30 2016
2016	National Science Foundation Panel Reviewer
2016-Present	Councilor, American Chemical Society, Iowa Local Section
2016	Co-Organized symposium, "Molecular Modeling of Surface-Mediated Electrochemical and Sorption Reactions" as part of the Geochemistry program for the Fall 2016 National Meeting of the American Chemical Society. (Co-organizers: Vitaly Alexandrov (University of Nebraska Lincoln) and Louise Criscenti (Sandia National Lab) Reviewed 6 journal manuscripts
2015	Co-Organized symposium, "Molecular-scale processes controlling reactivity at mineral-water
2014	interfaces" as part of the Division of Colloid and Surface Chemistry section program for the Spring 2015 National Meeting of the American Chemical Society. (Co-organizers: Dr. Sang Soo Lee (Argonne National Lab) and Dr. Anastasia Ilgen (Sandia National Lab))
2014	Reviewed 6 journal manuscripts
2013	Reviewed 9 journal manuscripts
2013	Co-Organized the (three ½ day session) symposium, "Behavior of Contaminants at Environmental Interfaces" as part of the Division of Colloid and Surface Chemistry section program for the Fall 2013 National Meeting of the American Chemical Society. (Co-organizer: Prof. Tori Z. Forbes)
2011	Total of 5 manuscripts reviewed for ACS and APS journals
2011-2014	Accepted appointment as 3-year term chair for the ACS Division of Colloid and Surface Chemistry continuing symposium of "Interfacial Chemistry and the Environment."
2011	Co-Organized the (four ½ day session) symposium, "Reactive Properties of Environmental Interfaces" as part of the Division of Colloid and Surface Chemistry section program for the Fall 2011 National Meeting of the American Chemical Society. (Co-organizer: Prof. S. C. Petitto, St. Cloud State University)
2011	Participant in the NSF Workshop on Nanomaterials in the Environment, held in Arlington VA June 28-29 2011
2010	Total of 4 manuscripts reviewed for ACS and APS journals
2010	Ad hoc reviewer of 1 Department of Energy proposal

Department

2021-2022	*Departmental Committee Assignments:* Executive Committee

	Graduate Education (chair) Annual Review (Bhattacherjee) *Other Departmental Service:* Director of Graduate Studies Faculty Forum Presentation: Overview of MPS ASCEND Solicitation from NSF
2020-2021	*Departmental Committee Assignments:* Executive Committee Graduate Education (chair) *Other Departmental Service:* Director of Graduate Studies Faculty Speaker, DEI Identity Week LGBTQ+ Discussion Physical Chemistry Overview presentation at Departmental Open House Events
2019-2020	*Departmental Committee Assignments:* Departmental Review Graduate Education Salary Committee Climate and Diversity Publicity and Alumni Relations Physical Chemistry Faculty Search *Other Departmental Service:* Director of Graduate Studies (effective Summer 2020) Physical Chemistry Overview presentation at Departmental Open House Events
2018-2019	*Departmental Committee Assignments:* Graduate Recruiting (chair) Climate and Diversity Salary Committee Publicity and Alumni Relations (chair) *Other Departmental Service:* Physical Chemistry Overview presentation at Departmental Open House Events
2017-2018	*Departmental Committee Assignments:* Graduate Recruiting Climate and Diversity Publicity and Alumni Relations *Other Departmental Service:* Physical Chemistry Overview presentation at Departmental Open House Events
2016-2017	*Departmental Committee Assignments:* Graduate Recruiting Graduate Student Awards & Fellowships Physical Chemistry/Informatics Faculty Search Publicity and Alumni Relations *Other Departmental Service:* Physical Chemistry Overview presentation at Departmental Open House Events
2015-2016	*Departmental Committee Assignments:* Facilities (research computing, shared instrumentation) Publicity and Alumni Relations Colloquium *Other Departmental Service:* Physical Chemistry Overview presentation at Departmental Open House Events
2014-2015	*Departmental Committee Assignments:* Facilities (research computing, shared instrumentation) Publicity and Alumni Relations

	Colloquium *Other Departmental Service:* Research Overview Presentation to First-Year Graduate Students Physical Chemistry Overview presentation at Departmental Open House Events
2013-2014 2012-2013 2011-2012	*Departmental Committee Assignments:* Publicity and Alumni Relations Colloquium *Other Departmental Service:* Research Overview Presentation to First-Year Graduate Students Physical Chemistry Overview presentation at Departmental Open House Events *Departmental Committee Assignments:* Library Committee Facilities (research computing, shared instrumentation) *Other Departmental Service:* Research Overview Presentation to First-Year Graduate Students TA Training event on the topic of professionalism *Departmental Committee Assignments:* Library Committee Other Departmental Service: Research Overview Presentation to First-Year Graduate Students
2010-2011	*Departmental Committee Assignments:* Library Committee *Other Departmental Service:* Research Overview Presentation to First-Year Graduate Students

College/University

College	
2022-2025	Faculty Senate, College of Liberal Arts & Sciences Group 3, three year term
2022	Applied Mathematical & Computer Sciences: Developed and delivered a series of five lectures (with hands-on activities) to introduce AMCS students to C++ programming (March-April 2022)
2022	Internal Reviewer, Physics and Astronomy Department (March 2022)
2021-2024	CLAS Diversity, Equity, and Inclusion Committee, member. (3 year term starting Fall 2021).
2021	Science Salaries Subcommittee, member, College of Liberal Arts and Sciences
2021	Career Boot Camp Planning Committee, member, College of Liberal Arts and Sciences.
2021	Completed Learning Outcomes and Assessment template for the Department of Chemistry, as assigned by the Graduate College.
2020*	Internal Reviewer, Physics and Astronomy Department *Delayed to Spring 2022 due to COVID-19
2018	CLAS Student Sustainability Showcase, presenter and panelist
2016	Developed and taught a First-Year Seminar: "Energy and the Environment" in the Fall 2016 Semester. Enrollment: 15. Delivered lectures on topics such as "Energy and Climate," "Alternative Energy Sources," and "Energy Efficient Buildings." As a class project, the students presented posters at a symposium held in the Chemistry Building.
University	
2013-Present	Campus Partner Facilitator for the Division of Diversity, Equity, and Inclusion (Formerly: Safe Zone Facilitator). Recent trainings delivered: Safe Zone II (2/22), Trans Awareness (9/21), Safe

	Zone II (8/21)
2012	OVPR MPSFP internal funding program, Reviewer
2011-2012	Represented UI at Statewide Annual Articulation Conference: Iowa's Public Colleges and Universities

TEACHING

Courses Taught at the University of Iowa

Term	Course#	Title	Ten-Day Enrollment	Final Enrollment
Fall 2021	CHEM:5091	Graduate Chemistry Orientation	42	
	CHEM:4480	Introduction to Molecular Modeling	12	
	CHEM:7999	Research in Chemistry	6	
Spring 2021	CHEM:6990	Research Seminar	9	9
	CHEM:7999	Research in Chemistry	6	6
Fall 2020	CHEM:5091	Graduate Chemistry Orientation	16	16
	CHEM:1110	Principals of Chemistry I	712	658
	CHEM:7999	Research in Chemistry	18	18
Spring 2020	CHEM:7999	Research in Chemistry	4	4
Fall 2019	CHEM:1120	Principles of Chemistry II	437	399
	CHEM:7999	Research in Chemistry	4	4
Spring 2019	CHEM:4432	Physical Chemistry II	13	12
	CHEM:5490	Seminar: Physical and Environmental Chemistry	14	14
	CHEM:7999	Research in Chemistry	6	6
Fall 2018	CHEM:4480	Introduction to Molecular Modeling	9	9
	CHEM:7999	Research in Chemistry	5	5
Spring 2018	CHEM:1110	Principles of Chemistry I	688	615
	CHEM:3994	Undergraduate Research	1	1
	CHEM:7999	Research in Chemistry	4	4
Fall 2017	CHEM:3994	Undergraduate Research	2	2
	CHEM:7999	Research in Chemistry	3	3
Spring 2017	CHEM:5433	Quantum and Computational Chemistry	9	9
	CHEM:3994	Undergraduate Research	2	2
	CHEM:7999	Research in Chemistry	2	2
Fall 2016	CHEM:4431	Physical Chemistry I	38	37
	CHEM:7999	Research in Chemistry	3	3
	CHEM:1000	First-Year Seminar	15	15
Spring 2016	CHEM:4431	Physical Chemistry I	28	28
	CHEM:7999	Research in Chemistry	4	4

Innovations in Teaching (Other Teaching Contributions)

Spring 2022	**AMCS:5900** Developed/Delivered 5 lecture series (with hands-on activities) to the Applied Mathematics and Computational Sciences (AMCS) program: Introduction to Programming in C++
Spring 2021	**CHEM:6990**, Created a 1 sh version of the Graduate Orientation Class for international students who started the program in January '21 owing to COVID impact.
Fall 2020	**CHEM:1110**, Member of the teaching team that implemented the new curriculum.
Fall 2020	**CHEM:5091**, New preparation, course delivered online owing to COVID impact.
Fall 2019	**CHEM:1120**, New preparation.
Spring 2019	**CHEM:4432**, New preparation.
Spring 2017	**CHEM:5433**, New preparation, first time this course was offered in the Department of Chemistry since before 2010.
Fall 2018	**CHEM:4480**, Redesigned the class to be 50% hands-on computational (held in computer lab) and 50% lecture.

Student Mentoring Summary

Term	Undergraduate Research Students	Graduate Research Students	Postdoctoral Fellows	Graduate Committees
Fall 2021	2	5	0	13
Spring 2021	1	6	0	12
Fall 2020	1	5	1	12
Spring 2019	1	5	1	14
Fall 2019	0	5	2	14
Spring 2018	0	5	2	13
Fall 2018	1	4	2	13
Spring 2017	1	4	2	
Fall 2017	1	4	2	
Spring 2016	0	5	2	
Fall 2016	0	5	2	

Student Mentoring

Graduate Students

Fall 2011-Spring 2016|	Witkin, Katie; *Ph.D. (complete)*
Spring 2013-Spring 2017	Huang, Xu; *Ph.D. (complete)*

Fall 2015-Fall 2020	Bjorklund, Jennifer; *Ph.D. (complete)*
Spring 2016-Summer 2021	Metz, Irene; *Ph.D. (complete)*
Fall 2016-Fall 2021	Jones, Diamond; *Ph.D. (complete)*
Fall 2017-Present	Hudson, Blake; *Ph.D. (in progress, post-comp)*
Fall 2017-Present	Augustine, Logan; *Ph.D. (in progress, post-comp)*
Fall 2020-Present	Sweet, Ameila; *Ph.D. (in progress)*
Fall 2021-Present	Rivera, Victoria; *Ph.D. (in progress)* Yang Chen; *Ph.D. (in progress)* Hung Nguyen; *Ph.D. (in progress)* Harindu Rajapaksha; *Ph.D. (in progress, co-advised with Forbes)*

Undergraduate Students

Spring 2019-Fall 2021	Hollar, Ethan; *BA (in progress)*
Fall 2021	Dahlen, Nicholas; *BS (in progress)*
Fall 2016-Fall2018	Spurgeon, Sidney; *BS, complete*

Postdoctoral Fellows

July 2017-Sept.	Abbaspour Tamijani, Ali; *subsequent position: Postdoc, Brown University.*
April 2016-April 2019	Bennett, Joseph; *current position: Assistant Professor, Department of Chemistry, University of Maryland Baltimore County.*
October 2015-August 2016	Chi-Ya Yang; *subsequent position: Postdoc, Ohio State University*
June 2013-February 2015	Sai Kumar Ramadugu; *current position: Assistant Research Scientist, High Performance Computing, University of Iowa.*

Teaching Table

Semester/Yr	Advisees		Courses Taught		New Required ACE Scores					
	Undergrad	Grad	Course	Students Enrolled	Instructor Used Time Well	Instructor comm. clearly	Teaching methods helped students learn	Learning materials facilitated student learning	Assessment aligned with objective	Help was available to students
Fall 2020	1	5	CHEM: 1110: 000A	185	4.80	4.40	4.30	4.90	4.50	4.90
			CHEM:	357	4.8	4.30	4.70	5.0	4.5	5.3

			1110: 000B							
			CHEM: 1110: 000C	368	5.3	4.9	5	5.3	5.2	5.5
			CHEM: 1110: 000D	157	5.1	4.5	4.8	5.2	5	5.3
			CHEM: 5091	16	5.6	5.8	5.8	5.7	5.8	5.9
					Instructor was effective	Work assigned wort-hwhile	Instruct-or support-ed student learning	Instructor communi-cated at a level appropriate to my under-standing	My ability to evaluate data, conclusions, and hypotheses has improves	I have developed my ability to explain scientific concepts
Fall 2019	1	4	CHEM: 1120 000A	145	5.00	5.10	5.10	4.9	5.1	5.2
			CHEM: 1120 000B	310	5.4	5.5	5.6	6.6	5.4	5.5
Spring 2019	1	6	CHEM: 4432: 000A	13	5.2	5.8	5.5	5		
			CHEM: 5490	14	5.8	5.8	5.8	5.8		
Fall 2018	1	5	CHEM: 4480	9	5.8	5.9	5.9	5.8		
Spring 2018	1	4	CHEM: 1110: 000A	287	5.1	5.2	5.2	5.1	5.0	5.0
			CHEM: 1110: 000B	435	5.1	5.2	5.4	5.2	5.0	5.1
Spring 2017	2	2	CHEM: 5542	9	5.0	4.8	5.5	5.5		
Fall 2016	1	3	CHEM: 1000: 005	15	5.0	5.0	5.0	5.0		
			CHEM: 4431	37	5.8	5.6	5.8	5.6		