

Bess Vlasisavljevich Ph.D.

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Research Experience and Appointments

Assistant Professor. University of South Dakota
May 2017–Present

Postdoctoral Research Assistant. Northwestern University
Advisor: Prof. Toru Shiozaki (now at QSimulate)
August 2015–May 2017
Area of Research: Method Development and Applications in Molecular Magnets

Postdoctoral Research Assistant. The University of California Berkeley
Advisor: Prof. Berend Smit (now at EPFL)
July 2013–July 2015
Area of Research: Quantum Chemistry and Molecular Simulations in Nanoporous Materials

Education

June 2013
Ph.D. in Chemistry. University of Minnesota - Twin Cities (GPA 3.872/4.00)
Advisor: Prof. Laura Gagliardi (now at the University of Chicago)
Thesis title: Quantum chemical studies of actinides and lanthanides: From small molecules to the nanoscale

March 2010
M.S. in Chemistry. University of Minnesota - Twin Cities (GPA 3.889/4.00)
Advisor: Prof. Laura Gagliardi
Thesis title: Analyzing systems containing multiple actinides with multiconfigurational methods

December 2007
B.A. in Chemistry. University of Minnesota - Morris (GPA 3.853/4.00)
Advisor: Prof. Joseph Alia

Peer-Reviewed Publications at USD

1. J. Murillo, R. Bhowmick, K. L. M. Harriman, A. Gomez-Torres, J. Wright, R. W. Meulenberg, P. Miró, A. J. J. Metta-Magana, **B. Vlasisavljevich***, and S. Fortier. Actinide arene-metalates: Ion pairing effects on the electronic structure of unsupported uranium-arene sandwich complexes *Chem. Sci.* 2021, Accepted ([link](#))
2. M. O. Gaylor, P. Miró, **B. Vlasisavljevich**, A. A. Suduweli Kondage, L. M. Barge, A. Omaran, P. Videau, V. A. Swenson, L. J. Leinen, N. W. Fitch, K. L. Cole, C. Stone, S. M. Drummond, K. Rageth, L. R. Dewitt, S.

- González Henao, and V. Karanauskus Plausible Emergence and Self Assembly of a Primitive Phospholipid from Reduced Phosphorus on the Primordial Earth *Orig. Life Evol. Biosph.* 2021, Accepted ([link](#))
3. Y. Pang, M. A. Ardagh, M. Shetty, A. Chatzidimitriou, G. Kumar, **B. Vlasisavljevič***, and P. Dauenhauer On the Spatial Design of Co-Fed Amines for Selective Dehydration of Methyl Lactate to Acrylates *ACS Catal.* 2021, 11, 9, 5718-5735. ([link](#))
 4. L. A. Mariano, **B. Vlasisavljevič**, and R. Poloni Improved Spin-State Energy Differences of Fe(II) Molecular and Crystalline Complexes via the Hubbard U-corrected Density *J. Chem. Theory Comput.* 2021, 17, 5, 2807-2816. ([link](#))
 5. K. A. Colwell, M. N. Jackson, R. M. Torres-Gavosto, S. Jawahery, **B. Vlasisavljevič**, J. M. Falkowski, B. Smit, S. C. Weston, and J. R. Long Buffered Coordination Modulation as a Means of Controlling Crystal Morphology and Molecular Diffusion in an Anisotropic Metal–Organic Framework *J. Am. Chem. Soc.* 2021, 143, 13, 5044–5052. ([link](#))
 6. W. Wu, J. Tehranchi De Hont, R. Parveen, **B. Vlasisavljevič***, and W. B. Tolman Sulfur-Containing Analogs of the Reactive $[\text{CuOH}]^{2+}$ Core *Inorg. Chem.* 2021, 60, 7, 5217-5223. ([link](#))
 7. V. M. Krishnan, D. Y. Shopov, C. J. Bouchey, W. D. Bailey, R. Parveen, **B. Vlasisavljevič***, and W. B. Tolman Structural Characterization of the $[\text{CuOR}]^{2+}$ Core *J. Am. Chem. Soc.* 2021, 143, 9, 3295-3299. ([link](#))
 8. L. Mariano, **B. Vlasisavljevič**, and R. Poloni Biased Spin-State Energetics of Fe(II) Molecular Complexes within Density Functional Theory and the Linear-Response Hubbard-U Correction *J. Chem. Theory Comput.* 2020, 16 (11), 6755-6762. ([link](#))
 9. T. Wiessner, S. A. Fosu, R. Parveen, N. Rath, **B. Vlasisavljevič***, and W. B. Tolman Ligand Effects on Decarbonylation of Palladium-Acyl Complexes *Organometallics* 2020, 39 (22), 3992-3998. ([link](#))
 10. S. C. Coste, T. J. Pearson, A. B. Altman, R. A. Klein, B. A. Finney, D. L. Brewé, M. Y. Hu, E. E. Alp, **B. Vlasisavljevič**, and D. E. Freedman Orbital Energy Mismatch Engenders High-Spin Ground States in Heterobimetallic Complexes *Chem. Sci.* 2020, 11, 9971–9977. ([link](#))
 11. K. Lee, P.-N. Lai, R. Parveen, C. M. Donahue, M. M. Wymore, B. A. Massman, **B. Vlasisavljevič**, T. S. Teets, and S. R. Daly. Modifying the Luminescent Properties of a Cu(I) Diphosphine Complex Using Ligand-Centered Reactions in Single Crystals, *Chem. Commun.* 2020, 56, 9110–9113. ([link](#))
 12. K. Lee, J. D. Culpepper, R. Parveen, D. Swenson, **B. Vlasisavljevič***, and S. R. Daly. Modifying Phosphorus(III) Substituents to Activate Remote Ligand-Centered Reactivity in Triaminoborane Ligands, *Organometallics* 2020, 39 (13), 2426–2533. ([link](#))
 13. A. Gamonal, C. Sun, A. L. Mariano, E. Fernandez-Bartolomé, E. Guerrero-SanVicente, **B. Vlasisavljevič**, J. Castells-Gil, C. Marti-Gastaldo, R. Poloni, R. Wannemacher, J. Cabanillas-Gonzalez, and J. Sanchez Costa Divergent Adsorption-Dependent Luminescence of Amino-Functionalized Lanthanide Metal-Organic Frameworks for Highly Sensitive NO_2 Sensors, *J. Phys. Chem. Lett.* 2020, 11, 3362–3368. ([link](#))
 14. J. W. Park, R. Al-Saadon, M. K. MacLeod, T. Shiozaki, and **B. Vlasisavljevič***. Multireference Electron Correlation Methods: Journeys Along Potential Energy Surfaces, *Chem. Rev.* 2020, 120, 13, 5878–5909. ([link](#))
 15. T. V. Fetrow, R. Bhowmick, A. J. Achazi, A. V. Blake, F. D. Eckstrom, **B. Vlasisavljevič***, and S. R. Daly. Chelating Borohydrides for Lanthanides and Actinides: Structures, Mechanochemistry, and Case Studies with Phosphinodboranates, *Inorg. Chem.* 2020, 59, 48–61. ([link](#))
 16. M. S. Fataftah, M. Krzyaniak, **B. Vlasisavljevič**, M. R. Wasielewski, J. M. Zadrozny, and D. E. Freedman. Metal–Ligand Covalency Enables Room Temperature Molecular Qubit Candidates, *Chem. Sci.* 2019, 10, 6707–6714. ([link](#))

17. A. Janda, L.-C. Lin, **B. Vlasisavljevič**, J. Van der Mynsbrugge, and A. T. Bell. Response to Impact of Zeolite Structure on Entropic-Enthalpic Contributions to Alkane Monomolecular Cracking: An IR Operando Study, *Dalton Trans.* 2019, 48, 3777–3785. ([link](#))
18. K. Lee, **B. Vlasisavljevič***, and S. R. Daly. Isolation of Ligand-Centered Borocations in Molybdenum Complexes Containing a Triaminoborane-Bridged Diphosphorus Ligand, *Dalton Trans.* 2019, 48, 3777–3785. ([link](#))
19. K. Lee, C. Kirkvold, **B. Vlasisavljevič***, and S. R. Daly. Ligand-Centered Boremium Reactivity in Triaminoborane-Bridge Diphosphine Complexes, *Inorg. Chem.* 2018, 57 (21), 13188–13200. ([link](#))
20. A. Wooles, D. P. Mills, F. Tuna, E. J. L. McInnes, G. T. W. Law, A. J. Fuller, F. Kremer, M. Ridgway, W. Lewis, L. Gagliardi, **B. Vlasisavljevič***, and S. T. Liddle. Uranium(III)-Carbon Multiple Bonding Supported by Arene δ -Bonding in Mixed-Valence Hexauranium Nanometre-Scale Rings., *Nature Commun.* 2018, 9, 2097. ([link](#))
21. A. Blake, T. Fetrow, Z. Theiler, **B. Vlasisavljevič***, and S. Daly. Homoleptic Uranium and Lanthanide Phosphinodiboronates *Chem. Commun.*, 2018, 54, 5602–5606. ([link](#))
22. M. Asgari, S. Jawahery, E. D. Bloch, M. R. Hudson, **B. Vlasisavljevič**, P. G. Boyd, B. Smit, C. M. Brown, J. R. Long, and W. L. Queen. An Experimental and Computational Study of CO₂ Adsorption in the Series of Sodalite-Type M-BT5 (M = Cr, Mn, Fe, Cu) Metal–Organic Frameworks Featuring Open Metal Sites. *Chem. Sci.*, 2018, 9, 4579–4588. ([link](#))
23. S. Fortier, J. Rolando Aguilar-Calderón, **B. Vlasisavljevič**, A. J. Metta–Magaña, A. G. Goos, and C. E. Botez. An *N*-Tethered Uranium(III) Arene Complex and the Synthesis of an Unsupported U-Fe Bond. *Organomet.* 2017, 36 (23), 4591–4599. ([link](#))

Peer-Reviewed Publications Prior to USD

24. M. L. Weichman, **B. Vlasisavljevič**, J. A. DeVine, N. S. Shuman, S. G. Ard, T. Shiozaki, D. M. Neumark, and A. A. Viggiano. Electronic Structure of SmO and SmO⁻ via Slow Photoelectron Velocity-Map Imaging Spectroscopy and Spin–Orbit CASPT2 Calculations. *J. Chem. Phys.* 2017, 147, 234311. ([link](#))
25. S. Coste, **B. Vlasisavljevič**, and D. Freedman. Magnetic Anisotropy from Main Group Elements: Halide versus Group 14 Elements. *Inorg. Chem.* 2017, 56 (14), 8195-8202. ([link](#))
26. S. Anderson, A. Gładysiak, P. G. Boyd, C. P. Ireland, P. Miéville, D. Tiana, **B. Vlasisavljevič**, P. Schouwink, W. Van Beek, K. J. Gagnon, B. Smit, and K. C. Stylianou. Formation Pathways of Metal–Organic Frameworks Proceeding Through Partial Dissolution of the Metastable Phase. *Cryst. Eng. Comm.* 2017, 19, 3407–3413. ([link](#))
27. **B. Vlasisavljevič**, J. Huck, Z. Hulvey, K. Lee, J. A. Mason, J. Neaton, J. R. Long, C. M. Brown, D. Alfe, A. Michaelides, and B. Smit. Performance of van der Waals Corrected Functionals for Guest Adsorption in the M₂(dobdc) Metal–Organic Frameworks. *J. Phys. Chem. C* 2017, 121 (21), 4139–4151. ([link](#))
28. S. Jawahery, C. M. Simon, E. Braun, M. Witman, D. Tiana, **B. Vlasisavljevič**, and B. Smit. Adsorbate-Induced Lattice Deformation in IRMOF-74 Series. *Nature Comm.*, 2017, 8, 13945. ([link](#))
29. A. Janda, **B. Vlasisavljevič**, B. Smit, L.-C. Lin, and A. T. Bell. Effects of Pore and Cage Topology on Thermodynamics of *n*-Alkane Adsorption at Brønsted Protons in Zeolites at High Temperature. *J. Phys. Chem C*, 2017, 121 (3), 1618-1638. ([link](#))

30. **B. Vlasisavljevič** and T. Shiozaki. Nuclear Energy Gradients for Internally Contracted Complete Active Space Second-Order Perturbation Theory: Multistate Extensions. *J. Chem. Theory Comput.* 2016, 12 (8), 3781-3787. ([link](#))
31. M. S. Fataftah, S. C. Coste, **B. Vlasisavljevič**, J. M. Zadronzny, and D. E. Freedman. Transformation of the Coordination Complex $[\text{Co}(\text{C}_3\text{S}_5)_2]^{2-}$ from a Molecular Magnet to a Potential Qubit. *Chem. Sci.*, 2016, 7, 6160-6166. ([link](#))
32. R. Mercado, **B. Vlasisavljevič**, L.-C. Lin, K. Lee, Y. Lee, J. A. Mason, D. Xiao, M. Gonzalez, M. Kapelewski, J. Neaton, and B. Smit. Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metal–Organic Frameworks. *J. Chem. Phys. C*, 2016, 120 (23), 12590-12604. ([link](#))
33. P. Miró, **B. Vlasisavljevič**, A. Gil, P. C. Burns, M. Nyman, and C. Bo. Self-assembly of Uranyl-peroxide Nanocapsules in Basic Peroxidic Environments. *Chem. Eur. J.*, 2016, 22 (25), 8571-8478. ([link](#))
34. A. Janda, **B. Vlasisavljevič**, L.-C. Lin, B. Smit, and A. T. Bell. Effects of Zeolite Structural Confinement on Adsorption Thermodynamics and Reaction Kinetics for Monomolecular Cracking and Dehydrogenation of *n*-Butane. *J. Am. Chem. Soc.* 2016, 138 (14), 4739-4756. ([link](#))
35. **B. Vlasisavljevič***, L. Andrews, X. Wang, Y. Gong, G. P. Kushto, and B. E. Bursten. Detection and Electronic Structure of Naked Actinide Complexes: Rhombic-Ring $(\text{AnN})_2$ Molecules Stabilized by Delocalized π -Bonding. *J. Am. Chem. Soc.* 2016, 138 (3), 893-905. ([link](#))
36. S. Tyler, S. Natoli, **B. Vlasisavljevič**, P. Fanwick, and T. Ren. Turning a New Leaf on Metal-TMC Chemistry: $\text{Ni}^{\text{II}}(\text{TMC})\text{Acetylides}$. *Inorg. Chem.* 2015, 54 (20), 10058-10064. ([link](#))
37. Z. Hulvey, **B. Vlasisavljevič**, J. A. Mason, E. Tsvision, T. P. Dougherty, E. D. Bloch, M. Head-Gordon, B. Smit, J. R. Long, and C. M. Brown. Critical Factors Driving the High Volumetric Uptake of Methane in $\text{Cu}_3(\text{btc})_2$. *J. Am. Chem. Soc.* 2015, 137 (33), 10816-10825. ([link](#))
38. W. S. Drisdell, R. Poloni, T. M. McDonald, T. A. Pascal, L. F. Wan, C. D. Pemmaraju, **B. Vlasisavljevič**, S. O. Odoh, J. B. Neaton, J. R. Long, D. Prendergast, and J. B. Kortright. Probing the Mechanism of CO_2 Capture in Diamine-Appended Metal–Organic Frameworks Using Measured and Simulated X-ray Spectroscopy. *Phys. Chem. Chem. Phys.*, 2015, 17, 21448-21457. ([link](#))
39. **B. Vlasisavljevič**, S. O. Odoh, A. L. Dzubak, S. K. Schnell, N. Planas, K. Lee, J. Neaton, B. Smit and L. Gagliardi. CO_2 Induced Phase Transitions in Diamine-Appended Metal–Organic Frameworks. *Chem. Sci.*, 2015, 6, 5177-5185. ([link](#))
40. J. S. Lee, **B. Vlasisavljevič**, D. K. Britt, J. A. Reimer, B. Smit, J. B. Neaton, J. R. Long, M. Haranczyk, and W. L. Queen. Understanding Small Molecule Interactions in Metal–Organic Frameworks: Coupling Experiment with Theory. *Adv. Mater.*, 2015, 27 (38), 5785-5796. ([link](#))
41. A. Janda, **B. Vlasisavljevič**, L.-C. Lin, S. M. Sharada, B. Smit, M. Head-Gordon, and A. T. Bell. Adsorption Thermodynamics and Intrinsic Activation Parameters for Monomolecular Cracking of *n*-Alkanes on Brønsted Acid Sites in Zeolites. *J. Phys. Chem. C*, 2015, 119 (19), 10427-10438. ([link](#))
42. J. Qui, **B. Vlasisavljevič**, L. Jouffret, K. Nguyen, J. E. S. Szymanowski, L. Gagliardi, and P. C. Burns. Cation Templating and Electronic Structure Effects in Uranyl Cage Clusters Probed by the Isolation of Peroxide-Bridged Uranyl Dimers. *Inorg. Chem.*, 2015, 54 (9), 4445-4455. ([link](#))
43. T. M. McDonald, J. A. Mason, X. Kong, E.D. Bloch, D. Gygi, A. Dani, V. Crocella, F. Giordanino, S. O. Odoh, W. S. Drisdell, **B. Vlasisavljevič**, A. L. Dzubak, R. Poloni, S. K. Schnell, N. Planas, K. Lee, T. A. Pascal, L. F. Wan, D. Prendergast, J. B. Neaton, B. Smit, J. B. Kortright, L. Gagliardi, S. Bordiga, J. A. Reimer, and J. R. Long. A Cooperative Insertion Mechanism for Efficient CO_2 Capture in Diamine-Appended Metal–Organic Frameworks. *Nature*, 2015, 519, 303-308. ([link](#))

44. L. Luo, L. Balhorn, **B. Vlasisavljević**, D. Ma, J. Choi, L. Gagliardi, and C. D. Frisbie. Hopping Transport and Diode Behavior in Long Donor-Acceptor Molecular Wires. *J. Phys. Chem. C*, 2014, 118 (46), 26485-26497. ([link](#))
 45. P. Miró, **B. Vlasisavljević**, A. L. Dzubak, S. Hu, C. J. Cramer, R. Spezia, and L. Gagliardi. Uranyl-Peroxide Nanocapsules in Aqueous Solution: Force Field Development and First Applications. *J. Phys. Chem. C*, 2014, 118 (42), 24730-24740. ([link](#))
 46. L. Andrews, X. Wang, Y. Gong, G. Kushto, **B. Vlasisavljević**, and L. Gagliardi. Infrared Spectra and Electronic Structure Calculations for NN Complexes with U, UN, and NUN in Solid Argon, Neon, and Nitrogen. *J. Phys. Chem. A*, 2014, 118, 5289-5303. ([link](#))
 47. L. Andrews, X. Wang, Y. Gong, **B. Vlasisavljević**, and L. Gagliardi. Infrared Spectra and Electronic Structure Calculations for the NUN(NN)₁₋₅ and NU(NN)₁₋₆ Complexes in Solid Argon. *Inorg. Chem.*, 2013, 52, 9989-9993. ([link](#))
 48. **B. Vlasisavljević**, P. L. Diaconescu, W. L. Lukens, Jr., L. Gagliardi, and C. C. Cummins. Investigations of the Electronic Structure of Arene-Bridged Diuranium Complexes. *Organomet.*, 2013, 32 (5), 1341-1352. ([link](#))
 49. **B. Vlasisavljević**, P. Miró, D. Ma, G. S. Sigmon, P. C. Burns, C. J. Cramer, and L. Gagliardi. Synthesis and Characterization of the First 2D Neptunyl Structure Stabilized by Side-on Cation-Cation Interactions. *Chem. Eur. J.* 2013, 19, 2937-2941. ([link](#))
 50. **B. Vlasisavljević**, P. Miró, D. Koballa, T. Todorova, C. J. Cramer, L. Gagliardi, S. Daly, and G. Girolami. Volatilities of Actinide and Lanthanide *N,N*-Dimethylaminodiboranate CVD Precursors: A DFT Study. *J. Phys. Chem. C* 2012, 116 (44), 23194-23200. ([link](#))
 51. **B. Vlasisavljević**, P. Miró, I. Infante, S. Liddle, C. J. Cramer, and L. Gagliardi. On the Nature of Actinide-Lanthanide-Metal Bonds in Heterobimetallic Compounds. *Chem. Eur. J.* 2011, 17, 8424-8433. ([link](#))
 52. X. Wang, L. Andrews, **B. Vlasisavljević**, L. Gagliardi. Combined Triple and Double Bonds to Uranium: The NUNH Uranimine Nitride Molecule Prepared in Solid Argon. *Inorg. Chem.* 2011, 50, 3826-3831. ([link](#))
 53. **B. Vlasisavljević**, L. Gagliardi, and P. C. Burns. Understanding the Structure and Formation of Uranyl Peroxide Nanoclusters by Quantum Chemical Calculations. *J. Am. Chem. Soc.* 2010, 132 (41), 14503-14508. ([link](#))
 54. **B. Vlasisavljević**, L. Gagliardi, X. Wang, B. Liang, L. Andrews, and I. Infante. U and P₄ Reaction Products: A Quantum Chemical and Matrix Isolation Spectroscopic Investigation. *Inorg. Chem.* 2010, 49, 9230-9235. ([link](#))
 55. H.-G. Cho, L. Andrews, **B. Vlasisavljević**, and L. Gagliardi. Infrared Spectra of Small Insertion and Methylene Complexes in Reactions of Laser-Ablated Palladium Atoms with Halomethanes. *Organomet.* 2009, 28 (24), 6871-6879. ([link](#))
 56. H.-G. Cho, L. Andrews, **B. Vlasisavljević**, and L. Gagliardi. Infrared Spectra of Small Insertion and Methylene Complexes in Reactions of Laser-Ablated Nickel Atoms with Halomethanes. *Organomet.* 2009, 28 (19), 5623-5632. ([link](#))
 57. J. Alia, **B. Vlasisavljević**, M. Abbot, H. Warneke, and T. Mastin. Prediction of Molecular Properties Including Symmetry from Quantum-Based Molecular Structural Formulas, VIF. *J. Phys. Chem. A* 2008, 112, 9784-9795. ([link](#))
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Grants

1. National Science Foundation (NSF) Center for Chemical Innovation (CCI): Center for Sustainable Polymers
 - Grant Role: Senior Investigator in large research center involving 19 senior investigators
 - Total Awarded: \$20,000,000
 - Total Awarded to Vlasisavljevic Research: \$395,436
 - August 2019 – July 2024
 2. NSF EPSCoR Track-2: Data Driven Material Discovery Center for Bioengineering Innovation
 - Grant Role: Senior Investigator in a multiple jurisdiction EPSCoR research center
 - Total Awarded: \$6,000,000
 - Total Awarded to Vlasisavljevic Research: \$173,000
 - August 2019 – July 2023
 3. Controlling Molecular Structure and Spin with Multiconfigurational Quantum Chemistry, Office of Science Department of Energy
 - Grant Role: Principal Investigator (Single Investigator Grant)
 - Total Awarded: \$600,000
 - Total Awarded to Vlasisavljevic Research: \$600,000
 - September 2018 – August 2023
 4. NSF Center for Sustainable Polymers Seed Grant: Ruthenium Catalyzed Decarbonylation Chemistry
 - Principal Investigator (Single Investigator Seed Grant)
 - Total Awarded: \$55,303
 - Total Awarded to Vlasisavljevic Research: \$55,303
 - September 2018 – July 2019
 5. NSF Industry-University Collaborative Research Centers (IUCRC) Planning Grant: Center for Solid-State Green Electric Power Generation and Storage (CEPS)
 - Co-Principal Investigator (Funds Supported the Submission of an Application for a Phase I Research Center).
 - Total Awarded: \$15,000
 - September 2018 – July 2019
 6. NSF Research Experiences for Undergrads (REU) Site: Undergraduate Research in Fluorine Chemistry, National Science Foundation. Grant Role: Supporting. (June 2018 -May 2022)
 - Grant Role: Supporting
 - Total Award: \$207,960
 - PI mentored one undergraduate student Summers 2018 and 2019.
 - June 2018 – May 2022
 7. University of South Dakota's Center for Teaching and Learning, Mobile Computing Initiative Grant, \$518, 2018
 8. University of South Dakota, College of Arts and Sciences, Faculty Travel Grant, \$500, 2018
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Presentations (45 Oral, 12 Poster)

Presentations while at USD, Full List Available Upon Request

25. **B. Vlasisavljevič.** Insights from Multireference Electron Correlation Methods in Transition Metal Chemistry. Presented in the Johns Hopkins Chemistry Department Seminar Series (September 7, 2021), Invited.
24. **B. Vlasisavljevič.** Computational Spectroscopy of Cr-Cr Bonds. Presented at the Department of Energy's Computational and Theoretical Chemistry (CTC) Virtual PI Meeting, (August 2, 2021), Invited.
23. **B. Vlasisavljevič.** Electronic structure and oxidation state in copper catalysts. Presented at the Molcas Developers Meeting (June 30, 2021). Contributed.
22. **B. Vlasisavljevič.** CASPT2 molecular geometries of dichromium complexes. Presented at the Great Lakes Regional Meeting (GLRM) of the American Chemical Society, (June 7, 2021). Contributed.
21. **B. Vlasisavljevič.** How Can High Performance Computing Help Design Sustainable Polymers?. Presented in the Great Plains Women in High Performance Computing Seminar Series (May 26, 2021), Invited.
20. **B. Vlasisavljevič.** Insights from Multireference Electron Correlation Methods in Transition Metal Chemistry. Presented in the South Dakota State University Department Seminar Series (April 16, 2021), Invited.
19. **B. Vlasisavljevič.** . Electronic structure and oxidation state in a copper catalyst. Presented in the American Chemical Society's Spring National Meeting (April 14, 2021). Contributed.
18. **B. Vlasisavljevič.** Electronic structure and oxidation state in copper catalysts. Presented in the University of Nebraska Omaha Department Seminar Series (April 12, 2021), Invited.
17. **B. Vlasisavljevič.** Electronic Structure and Oxidation State in Copper Catalysts. Presented in the Physical, Theoretical, and Computational Chemistry (PTC) Virtual Seminar Series (March 9, 2021), Invited.
16. **B. Vlasisavljevič.** Understanding Sustainable Polymers with Computational Chemistry. Presented in the USD Office of Sponsored Research (ORSP)'s Brown Bag Lunch Series, Virtual, (March 9, 2021), Invited.
15. **B. Vlasisavljevič.** Ligand Effects on Decarbonylation of Palladium-Acyl Complexes. Presented at the 5th International Conference on Catalysis and Chemical Engineering (CCE), Virtual, (February 25, 2021), Invited.
14. **B. Vlasisavljevič.** CASPT2 Molecular Geometries of Transition Metal Complexes. Presented at the ACS Sioux Valley Local Section's Fall Research Symposium, Virtual, (September 21, 2020), Contributed.
13. **B. Vlasisavljevič.** CASPT2 Molecular Geometries of Transition Metal Complexes. Presented at the University of South Dakota, Chemistry Department Seminar Series, (September 21, 2020), Invited.
12. **B. Vlasisavljevič.** CASPT2 Molecular Geometries and Electronic Structures of Transition Metal Complexes. Presented at the Department of Energy's Computational and Theoretical Chemistry (CTC) Virtual PI Meeting, (July 16, 2020), Invited.
11. **B. Vlasisavljevič.** CASPT2 Molecular Geometries of Late Transition Metal Complexes. Presented at the Virtual 260th American Chemical Society National Meeting. Oral Presentation On-Demand (August 17–20, 2020), Contributed.
10. **B. Vlasisavljevič.** Ligand-Centered Borenum Reactivity in Triaminoborane-Bridged Diphosphine Complexes. Presented at the Virtual 260th American Chemical Society National Meeting. Oral Presentation On-Demand (August 17–20, 2020), Contributed.

9. **B. Vlasisavljevič.** CASPT2 Molecular Geometries and Electronic Structures of Transition Metal Complexes. Presented at the 258th American Chemical Society National Meeting, San Diego, CA. (August 27, 2019), Invited.
 8. **B. Vlasisavljevič.** Electronic Structure of Uranium Arene Interactions. Presented at the Midwest Regional Meeting, Ames, IA. (October 23, 2018), Invited.
 7. **B. Vlasisavljevič.** Methane Storage in the $\text{Cu}_3(\text{btc})_2$ Metal-Organic Framework. Presented at the Department Seminar at University of Minnesota Morris, Morris, MN. (September 25, 2018), Invited.
 6. **B. Vlasisavljevič.** Methane Storage in the $\text{Cu}_3(\text{btc})_2$ Metal-Organic Framework. Presented at the Department Seminar at St. Olaf University, Northfield, MN. (April 19, 2018), Invited.
 5. **B. Vlasisavljevič.** Predictive Simulations of the Electronic Structure of Inorganic Molecules. Presented at the Computer Science Departmental Seminar series at the University of South Dakota, Vermillion, SD (April 4, 2018), Invited.
 4. **B. Vlasisavljevič.** Electronic Structure of Uranium Arene Interactions. Presented at the 255th ACS National Meeting, New Orleans, LA. (March 22, 2018), Invited.
 3. **B. Vlasisavljevič.** Methane Storage in the $\text{Cu}_3(\text{btc})_2$ Metal-Organic Framework. Presented at the Department Seminar at Winona State University, Winona, MN. (September 29, 2017), Invited.
 2. **B. Vlasisavljevič.** Electronic Structure of Single Molecule Magnets. Presented at the ACS Great Lakes Regional Meeting, Fargo, ND. (June 26, 2017), Invited.
 1. **B. Vlasisavljevič.** Electronic Structure of Single Molecule Magnets. Presented at the 253rd American Chemical Society National Meeting, San Francisco, CA. (April 2nd, 2017), Invited.
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Advising

Postdoctoral Researchers

- **Jorge Barroso** September 2021 to present.
- **Sabyasachi Roy Chowdhury** January 2021 to present.
- **Riffat Parveen.** June 2019 to June 2021. Current Position: Assistant professor, Department of Chemistry, Government College University, Lahore, Pakistan
- **Brian Finney.** September 2018 to June 2020.

Graduate Students

- **Kh Mahfuzul Alam,** Master's Student, January 2021 to present.
- **Parisa Fasihianifard,** Master's Student, November 2020 to present.
- **Ashen Suduweli Kondage,** Master's Student, November 2019 to August 2021. (co-advised with Prof. Pere Miró) MS defense scheduled December 2021.
- **Samuel Fosu,** PhD Student, November 2018 to present. MS Awarded 2020
- **Rina Rani Bhowmick,** PhD Student, November 2018 to present. MS Awarded 2020
- **Megan Bruns,** PhD Student, January 2018 to August 2018.

Undergraduate Students

- **Christina Nguyen** USD undergraduate student, Summer 2021 to present.
 - **Emma Saucerman** USD undergraduate student, Spring 2021 to present.
 - **Clara Kirkvold** USD undergraduate student. October 2017 to August 2020. Goldwater Scholar, NSF GRFP honorable mention in 2019, and NSF GRFP recipient in 2020. Supported by the NSF REU at USD for one summer, supported by the Department of Energy the second summer, and by the South Dakota Governor's Center for Functional Fluorinated Materials during the final summer. Participated in research during the academic year as well. Currently in graduate school at the University of Minnesota.
 - **MaKenna Koble**, Augustana undergraduate student, NSF REU summer student, Summer 2019. Current graduate student at the University of Minnesota.
 - **Andrew Reuter** St. Olaf undergraduate student, NSF REU summer student, Summer 2018. Completed his MS degree following his graduation from St. Olaf and his working in industry.
 - **Haley Rust**. USD undergraduate student. August 2017 to May 2018. (co-advised with Prof. Pere Miró) Graduated and applying for medical school or DO programs.
 - **Zachary Hansen**. undergraduate student. August 2017 to May 2018. (co-advised with Prof. Pere Miró)
 - **Ethan Hare**. undergraduate student. August 2017 to May 2018. (co-advised with Prof. Pere Miró) Graduate school in Biology at Auburn University.
 - **Taylor Pickthorn**. St. John's undergraduate student, NSF REU summer student. Summer 2017. (co-advised with Prof. Pere Miró)
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Teaching Experience

- Chem 106L: Survey of Chemistry I Lab, University of South Dakota (Fall 2018 (2 sections), Fall 2019 (2 sections), Fall 2020 (2 sections), Fall 2021 (1 section))
 - Chem 107L: Survey of Chemistry II Lab, University of South Dakota (Spring 2020 (1 section))
 - Chem 112L: General Chemistry I Lab, University of South Dakota (Fall 2017 (4 sections))
 - Chem 114L: General Chemistry II Lab, University of South Dakota (Spring 2021 (2 sections))
 - CHEM 544/444: Physical Chemistry II, University of South Dakota (Spring 2018, Spring 2019, Spring 2020, Spring 2021)
 - CHEM 542/442: Physical Chemistry I, University of South Dakota (Fall 2018, Fall 2020)
 - CHEM 442L: Physical Chemistry I, University of South Dakota (Spring 2020)
 - CHEM 744: Advanced Physical Chemistry, University of South Dakota (Fall 2019, Fall 2021)
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Awards

- President's Research Excellence Award, University of South Dakota, 2020
 - Overend Award for Graduate Research in Physical Chemistry. 2012–2013
 - University of Minnesota Graduate School Doctoral Dissertation Fellowship. 2012–2013
 - Bunsen and Beaker Award for Outstanding Presentation at the 2011 Chemistry Graduate Student Research Symposium. March 2011
 - Department of Chemistry Excellence in Graduate Studies Fellowship. 2010–2011
 - 60th Annual Lindau Nobel Laureates Meeting Participant. June 2010
 - Lester C. and Joan M. Krogh Endowed Fellowship, University of Minnesota - Twin Cities. 2008–2009
 - Scholar of the College, University of Minnesota - Morris. Spring 2008
 - Minnesota Air National Guard Aerial Port Squadron Airman of the Year - 2005, 2008
 - University of Minnesota - Morris Dean's List. Fall 2002, Spring 2003, Fall 2004, Spring 2005, Spring 2007, and Fall 2007.
 - Recipient of the Presidential and Chancellor's Scholarship, University of Minnesota, Morris. September 2002–December 2007
 - Valedictorian, St. Bernard's High School, St. Paul, MN. May 2002.
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Memberships

- American Chemical Society. January 2008 to Present
 - Member Number: 2435628
 - Member of the COMP Division and ACS Sioux Valley Local Section
 - American Chemical Society, Sioux Valley Local Section. August 2017 to present.
(Secretary: September 2019 – Present)
 - American Physical Society. January 2019 to Present
 - Graduate Student Workshop Committee, University of Minnesota. January 2010 – June 2013
(Chair: Jan 2011 – April 2013)
 - Association of Women Chemists, Northwestern University. August 2015 to Present
 - Women in Science and Engineering, University of Minnesota. September 2008 – June 2013
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Service

- Secretary of the Sioux Valley Local Section of the American Chemical Society (September 2019 to Present)
- Science Outreach Officer of the Eastern South Dakota Section of the Graduate Women in Science (GWIS) (June 2021 to Present)
- Member of the College of Arts and Sciences Strategic Planning Task Force (September 2021 to Present)
- Member of the Department of Chemistry's Graduate Admissions Committee (March 2021 to Present)
- College of Arts and Sciences Math and Science Division Secretary (September 2020 to Present)
- Advisor to the University of South Dakota's Chemistry Club (September 2018 to September 2020)
- College of Arts and Sciences Curriculum and Instruction Committee (September 2019 to May 2021)
- College of Arts and Sciences Harrington Committee (September 2018 to May 2020)
- University of South Dakota Exit Interview Task Force (Fall 2018)
- Instructor at a chemistry workshop at the Nebraska Indian Community College (NICC). Co-organized presentation and hands on exercises on computational chemistry.
- Participant in the Letters to a Pre-Scientist Program (pairs scientists with middle school students as pen pals). September 2012 to May 2017, August 2020 to Present
- Spoke at "Profs and Profs" outreach event hosted by the Society of Women Engineers (SWE) for undergraduate students. March 7th, 2013
- Volunteered at "See yourself in CSE" outreach events hosted by the Society of Women Engineers (SWE) for high school girls. November 5th, 2011 and February 25th, 2012
- Exploring Careers in Engineering and Physical Sciences Program for high school students. June 15, 2011
- Women in Science and Engineering's Cool Chemistry Event for middle school girls. April 17th, 2010 and April 30th, 2011

Last updated: September 30, 2021