Brent P. Krueger
Annotated Curriculum Vitae

Hope College, Department of Chemistry
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ACADEMIC POSITIONS AND AWARDS

2014–	Professor of Chemistry, Hope College
2013–	Schaap Research Fellow, Hope College
2021	Ruth and John Reed Faculty Achievement Award, Hope College
2007–14	Associate Professor of Chemistry, Hope College
2013	Visiting Scholar, University of Florida, Gainesville, FL
2007–08	Senior Research Associate, The Scripps Research Institute, La Jolla, CA
2004–07	Towsley Research Scholar, Hope College
2001–07	Assistant Professor of Chemistry, Hope College

EDUCATION AND TRAINING

1999–01	Postdoctoral Fellow, Department of Pharmaceutical Chemistry, University of California at San Francisco. Research Advisor: Professor Peter A. Kollman.
1999	Dutch Visiting Research Fellow, Department of Physics and Astronomy, Vrije Universiteit, Amsterdam, The Netherlands. Research Advisor: Professor Rienk van Grondelle.
1999	Ph.D. in Physical Chemistry, The University of Chicago, Chicago, IL. Dissertation Title: *The Role of Carotenoids in Bacterial Light Harvesting.* Graduate Research Advisor: Professor Graham R. Fleming.
1994	M.S. in Physical Chemistry, The University of Chicago.
1993	B.S. in Chemistry and Physics, *summa cum laude*, Truman State University, Kirksville, MO.

RESEARCH SUPPORT

Total funding since 2001 (since tenure review in parenthesis):

- 33 (24) monetary awards totaling $ 2,720,807 ($ 2,213,578).
- Sole PI or lead PI on 17 (14) of those awards totaling $ 1,334,903 ($ 1,254,283).

Selected awards since 2010:

2020   Michigan Department of Environment, Great Lakes, and Energy. *Implementation of digital droplet PCR technology for SARS-CoV-2 testing in wastewater in Ottawa and Allegan Counties.* ($493,605 plus instrumentation valued at $192,314) $ 685,919

2019–22   National Science Foundation. *MRI: Acquisition of a High Performance Computing Cluster for Undergraduate Chemistry Research and Teaching by the Midwest Undergraduate Computational Chemistry Consortium (MU3C).* $ 400,400.

2018–21   Department of Education. *FIPSE: Expanding the LibreTexts Project into the Next-Generation Hub for Construction, Dissemination, and Usage of Open Educational Resource Textbooks.* $ 161,691.
Part of a multi-institution grant led by Delmar Larsen totaling $ 4,949,843.

2015–18   National Science Foundation. *IUES: Collaborative Research: Developing and Assessing Effective Cyberlearning within the STEMWiki Hyperlibrary.* $ 35,741.
Part of a multi-institution grant led by Delmar Larsen totaling $ 574,992.

2015–17   Hope College-Howard Hughes Medical Institute Course Research Experiences Grant. *Programming Foundations with Application Modules.* $ 25,000.

2011–15   National Science Foundation. *RUI: Quantifying Fluorescent Probe Dynamics in FRET Experiments by Combining Single-Molecule and Bulk Spectroscopies with Molecular Dynamics and Quantum Mechanics Simulations.* $ 385,000.

2010–14   National Science Foundation. *MRI: Acquisition of a Computer Cluster for Undergraduate Chemistry Research and Teaching by the Midwest Undergraduate Computational Chemistry Consortium (MU3C).* $ 299,942.

SUMMARY OF RESEARCH WITH UNDERGRADUATE STUDENTS

- Mentored 65 Hope College undergraduate students and 1 postdoc in research.
- Additionally mentored 5 external undergraduate students along with 5 high school students and 2 high school teachers in summer research at Hope College.
- 8 Hope undergraduates are co-authors on 5 peer-reviewed journal articles.
- 9 additional Hope undergraduates are co-authors on work currently in preparation.
- 23 Hope undergraduates have given 32 research presentations at national and international meetings.
- 37 Hope undergraduates and 2 high school students have given 103 research presentations at regional meetings.
- Every student gives presentations at local seminars/meetings.

Overall H-index 17. H-index of Hope College work 8. Top two papers with Hope College undergraduates have 118 & 105 citations. (as of Jan 2021)

Articles Published Since Tenure Review
(Hope College undergraduate co-authors <u>underlined</u>)

1. Diarrhea prevalence in a randomized, controlled prospective trial of point-of-use water filters in homes and schools in the Dominican Republic. Nathan Tintle, Kristin Van De Griend, Rachel Ulrich, Randall D. Wade, <u>Tena M. Baar</u>, Emma Boven, <u>Carolyn E. A. Cooper</u>, Olivia Couch, <u>Lauren Eekhoff</u>, <u>Benjamin Fry</u>, <u>Grace K. Goszkowicz</u>, <u>Maya A. Hecksel</u>, Adam Heynen, <u>Jade A. Laughlin</u>, <u>Sydney M. Les</u>, <u>Taylor R. Lombard</u>, B. Daniel Munson, <u>Jonas M. Peterson</u>, <u>Eric Schumann</u>, <u>Daniel J. Settecerri</u>, <u>Jacob E. Spry</u>, <u>Matthew J. Summerfield</u>, <u>Meghana Sunder</u>, <u>Daniel R. Wade</u>, Caden G. Zonnefeld, Sarah A. Brokus, Francesco S. Moen, Adam D. Slater, Jonathan W. Peterson, Michael J. Pikaart, Brent P. Krueger and Aaron A. Best. *Tropical Medicine and Health,* 49:1 (2021). DOI: 10.1186/s41182-020-00291-y

2. Indocyanine Dyes Approach Free Rotation at 3' Terminus of A-RNA: A Comparison with the 5' Terminus and Consequences for Fluorescence Resonance Energy Transfer. P. Milas, B.D. Gamari, L. Parrot, B.P. Krueger, S. Rahmanseresht, J. Moore, and L.S. Goldner. *J. Phys. Chem. B*, 117, 8649-8658 (2013). DOI: 10.1021/jp311071y.

3. Developing a Regional Computational Chemistry Consortium Through Undergraduate Research Conferences. K.T. Kuwata, D. Kohen, B.P. Krueger, and W.F. Polik. *CUR Quarterly*, **32**, 9-14. (2012).

4. Using Molecular Dynamics and Quantum Mechanics Calculations to Model Fluorescence Observables. <u>A. L. Speelman</u>, A. Muoz-Losa, <u>K. L. Hinkle</u>, <u>D. B. VanBeek</u>, B. Mennucci, and B. P. Krueger. *J. Phys. Chem. A.*, **115**, 3997-4008. (2011). DOI: 10.1021/jp1095344.

5. A Thermodynamic Exploration of Eosin-Lysozyme Binding: A Physical Chemistry and Biochemistry Laboratory Experiment. <u>A.J. Huisman</u>, <u>L.R. Hartsell</u>, B.P. Krueger, and M.J. Pikaart. *J. Chem. Educ.*, **87**, 299-302 (2010). DOI: 10.1021/ed800075k.

6. Fretting about FRET: Failure of the Ideal Dipole Approximation. A. Muñoz-Losa, C. Curutchet, B. P. Krueger, <u>L. R. Hartsell</u>, and B. Mennucci. *Biophys. J.*, **96**, 4779–4788 (2009). DOI: 10.1016/j.bpj.2009.03.052.

7. Theoretical Studies of Short Polyproline Systems: Recalibration of a Molecular Ruler. E. Dolghih, W. Ortiz, S. Kim, B. P. Krueger, J. L. Krause, and A. E. Roitberg. *J. Phys. Chem. A*, **113**, 4639–4646 (2009). DOI: 10.1021/jp811395r.

Articles Based on Work at Hope College Prior to Tenure Review

8. Hybrid Molecular Dynamics-Quantum Mechanics Simulations of Condensed Phase Spectral Properties: Evaluation of Simulation Parameters. <u>M. C. Zwier</u>, <u>J. M. Shorb</u>, and B. P. Krueger. *J. Comput. Chem.*, **28**, 1572–1581 (2007) DOI: 10.1002/jcc.20662.

9. Fretting about FRET: Correlation between κ and R. <u>D.B. VanBeek</u>, <u>M.C. Zwier</u>, <u>J.M.</u>

<u>Shorb</u>, and B.P. Krueger. *Biophys. J.* **92**, 4168–4178 (2007) DOI: 10.1529/biophysj.106.092650.

10. Structural Fluctuations and Excitation Transfer Between Adenine and 2-Aminopurine in Single-Stranded Deoxytrinucleotides. J.M. Jean and B.P. Krueger. *J. Phys. Chem. B.* **110**, 2899-2909 (2006) DOI: 10.1021/jp054755+.

11. Energy Transfer in the Nanostar: The Role of Coulombic Coupling and Dynamics. W. Ortiz, B.P. Krueger, V.D. Kleiman, J.L. Krause, and A.E. Roitberg. *J. Phys. Chem. B.* **109**, 11512-11519 (2005). 10.1021/jp050611j.

12. Photochemical Reaction. G. R. Fleming, B.P. Krueger , and J. W. Longworth. In: *Encyclopedia Britannica Online*. https://www.britannica.com/science/photochemical-reaction

Articles Based on Postdoctoral Work

13. Energy Transfer in Light-Harvesting Complexes LHCII and CP29 of Spinach Studied with Three-Pulse Echo Peak Shift and Transient Grating. J.M. Salverda, M. Vengris, B.P. Krueger, G.D. Scholes, A.R. Czarnoleski, V. Novoderezhkin, H. van Amerongen, and R. van Grondelle. *Biophys J.* **84**, 450-465 (2003).

14. Energy transfer in the peridinin-chlorophyll-a-protein of Amphidinium carterae studied by polarized absorption measurements. S.S. Lampoura, B.P. Krueger, I.H.M. Van Stokkum, J.M. Salverda, C.C. Gradinaru, D. Rutkauskas, R.G. Hiller, R. Van Grondelle. *Int.J.Mod.Phys. B.* **15,** 3849-3852 (2001).

15. Molecular Dynamics Simulations of a Highly-Charged Peptide from an SH3 Domain: A Possible Sequence-Function Relationship. B.P. Krueger and P. A. Kollman. *Proteins.* **45**, 4-15 (2001).

16. Energy Transfer in the Peridinin Chlorophyll-*a* Protein of *Amphidinium carterae* Studied by Polarized Transient Absorption and Target Analysis. B.P. Krueger, S.S. Lampoura, I.H.M. van Stokkum, E. Papagiannakis, J.M. Salverda, C.C. Gradinaru, <u>D. Rutkauskas</u>, R.G. Hiller, and R. van Grondelle. *Biophys. J.* **80**, 2843-2855 (2001).

Articles Based on Graduate Work

17. Two-Photon Excitation Spectrum of Light-Harvesting Complex II and Fluorescence Upconversion after One- and Two-Photon Excitation of the Carotenoids. P.J. Walla, J. Yom, B.P. Krueger, and G.R. Fleming. *J. Phys. Chem. B.* **104**, 4799-4806 (2000).

18. Ultrafast Energy Transfer in LHC-II Revealed by Three-Pulse Photon Echo Peak Shift Measurements. R. Agarwal, B.P. Krueger, G.D. Scholes, M. Yang, J. Yom, L. Mets, and G.R. Fleming. *J. Phys. Chem. B.* **104**, 2908-2918 (2000).

19. Observation of the S_1 State of Spheroidene in LH2 by Two-Photon Fluorescence Excitation. B.P. Krueger, J. Yom, P.J. Walla, and G.R. Fleming. *Chem. Phys. Lett.* **310**, 57-64 (1999).

20. Carotenoid Mediated B800-B850 Coupling in LH2. B.P. Krueger, G.D. Scholes, I.R. Gould, and G.R. Fleming. *PhysChemComm.* **2**, 34-40 (1999). DOI: 10.1039/a903172c http://www.rsc.org/Publishing/Journals/QU/article.asp?doi=a903172c.

21. The Light Harvesting Process in Purple Bacteria. B.P. Krueger, G.D. Scholes, J.-Y. Yu, and G.R. Fleming. *Acta Physica Polonica A* (Special Issue: Jablonski Centennial Conference on Luminescence and Photophysics, Torun, July 23-27, 1998), **95**, 63-83 (1999).

22. Fluorescence Upconversion and *ab initio* Studies of the Light-Harvesting Function of Carotenoids in Bacterial Light-Harvesting Antenna. B.P. Krueger, G.D. Scholes, I.R. Gould, and G.R. Fleming. In: *Ultrafast Phenomena XI*, eds. T. Elsaesser, J.G. Fujimoto, D.A. Wiersma, W. Zinth, Springer-Verlag, Berlin Heidelberg, p.666-668 (1998).

23. Calculation of Couplings and Energy Transfer Pathways Between the Pigments of LH2 by the *ab initio* Transition Density Cube Method. B.P. Krueger, G.D. Scholes, and G.R. Fleming. *J. Phys. Chem. B.* **102**, 5378-5386 (1998). And correction: **102**, 9603 (1998).

24. Electronic Excitation Transfer from Carotenoid to Bacteriochlorophyll in the Purple Bacterium *Rhodopseudomonas acidophila*. B.P. Krueger, G.D. Scholes, R. Jimenez, and G.R. Fleming. *J. Phys. Chem. B.* **102**, 2284-2292 (1998).

25. Soluble Synthetic Multi-Porphyrin Arrays. 2. Photodynamics of Energy-Transfer Processes. J-S. Hsiao, B.P. Krueger, R.W. Wagner, J.K. Delaney, D.C. Mauzerall, G.R. Fleming, J.S.Lindsey, D.F. Bocian, and R.J. Donohoe. *J. Am. Chem. Soc.* **118**, 11181-11193 (1996).

Scholarly Work Currently In Progess

26. Force-Field Parameters to Describe GFP and related Chromophores. <u>D.L. Blood</u>, <u>A.M. Rosnik</u>, B.P. Krueger. *Expected submission, late 2020*

27. Monovalent Ion Parameters Suitable for Use with the Optical Point Charge Water Model. <u>D.E. Clark</u>, <u>J. C. Dood</u> and B. P. Krueger. *In Progress.*

28. Descriptions of Common FRET Probes for Use with AMBER. <u>A.M. Stevenson</u>, <u>A.E. Cook</u>, <u>D.A. Paul</u>, <u>B.A. Leland</u>, <u>A.L. Speelman</u>, <u>A.A. Cassabaum</u>, <u>C.A. Gobrogge</u>, <u>D.W. Summers</u>, <u>A.S. Ortega</u>, B.P. Krueger. *In progress.*

29. Identification and Expression Patterns of the slc7a11 Gene in Zebrafish. <u>N.A. Ladd</u>, <u>M. Solórzano</u>, <u>K.C. Franz</u>, <u>C.O. Da Silva</u>, L.A. Chase, A.P. Putzke, and B.P. Krueger. *In Progress.*

Books/Editorial Work

Associate Editor & Preface Author (with G.C. Walker): *Biological Nanoscience*, Vol. 2 of *Comprehensive Nanoscience and Technology*. Eds. in Chief: David L. Andrews, Gregory D. Scholes, and Gary P. Wiederrecht. Academic Press, Amsterdam. 2011. ISBN: 978-0-12-374390-9.

Other Publications

hocker: A Python 3 wrapper to enable secure Docker container usage in an HPC cluster. Zachary Snoek, Anna Prins, Brian Slenk, Dan Yonker, Dean Thayer, Jeff Pestun, Brent P. Krueger. https://github.com/hopehpc/hocker. First released Sept 2018.

AMBER Advanced Tutorials A1: Setting up an advanced system (including charge derivation). <u>B.A. Leland</u>, <u>D.A. Paul</u>, B.P. Krueger, and R.W. Walker. *AMBER Tutorials Website.* http://ambermd.org/tutorials/advanced/tutorial1/. First posted in 2008.

PRESENTATIONS

Invited Talks

1. "Two stories about water quality: Lake Macatawa and Global Drinking Water", Grace Episcopal Church Creation Care Group Sunday Forum Series. Holland, MI 2 February 2020.

2. "A Research Carol: Stories of Research Past, Present, and Future", Professor Graham R. Fleming's 70th Birthday Symposium, Department of Chemistry, The University of Chicago, 15 July 2019.

3. "Day1 Research Communities", Natural and Applied Sciences Pedagogy Innovation Lunch, Hope College, Holland, MI, 28 February 2019. (with C.M. Mader, B.E. Bodenbender, and J. Krupczak)

4. "Fretting about FRET: Modeling Fluorescence Observables", FRET and Beyond Conference, Warsaw, Poland, 3 May 2018.

5. "Two tales of molecular dynamics parameters: Fluorescent protein chromophores and aqueous ions", Macalester College Chemistry Department Seminar Series, St. Paul, MN. 22 March 2017.

6. "Progress in Parameters: Fluorescent Protein Chromophores and Aqueous Ions for the OPC Water Model", AMBER Developers Meeting. San Diego Supercomputer Center, San Diego, CA 19 March 2016.

7. "Fretting about FRET: Using simulation to bridge the gap between theory and experiment" Michigan State University Physical Chemistry Seminar, East Lansing, Michigan, 1 December 2015.

8. "Fretting about FRET: Examining the Underlying Assumptions." Principles of Single Molecule Techniques Workshop, University of Michigan, Ann Arbor, Michigan. 13-14 October 2014.

9. "Multi-region QM/MM Simulations in AMBER", AMBER Developers' Meeting. Stony Brook, NY. 16 January 2014.

10. "Dynamic Textbook Development." Hope College Retirees. 20 Nov 2013.

11. "Single-Molecule Fluorescence Instrumentation: Optical and Electronic Considerations." Amherst College, O'Hara research group. 1 May 2013.

12. "Computational Science and Modeling Across the Curriculum." Midwest P3 Workshop, Preparing Postdocs for Undergraduate Faculty Careers in Chemistry, Hope College, 11 April 2013.

13. "Fretting about FRET: Using simulation to bridge the gap between theory and experiment." University of Barcelona, Department of Physical Chemistry. 1 March

2013.

14. "Fretting about FRET: Bridging the gap between experiment and theory." Bowdoin College, Department of Chemistry. 7 Feb 2013.

15. "Single-Molecule Fluorescence Instrumentation." University of Florida, Roitberg group meeting. 24 January 2013.

16. "Fretting about FRET: Examining the Underlying Assumptions." University of Florida, Quantum Theory Project. 23 January 2013.

17. "Introducing Molecular Modeling to High School Students and Teachers." ChemEd 2011 International Conference, Western Michigan University. 27 July 2011. Talk given together with undergraduate student Cortney Kimmel.

18. "Fretting about FRET: A Detailed Look at Several FRET Approximations." Gentex Corporation, Chemistry Department. 5 May 2011.

19. "Fretting about FRET: A Detailed Look at Several FRET Approximations." Western Kentucky University, Department of Physics. 2 May 2011.

20. "Computational Science and Modeling Across the Curriculum." Midwest P_3 Workshop, Preparing Postdocs for Undergraduate Faculty Careers in Chemistry, Hope College, 6 April 2011.

21. "Fretting about FRET: A Detailed Look at Several FRET Approximations." 51st Sanibel Symposium, St. Simons, GA. 1 March 2011.

22. "Fretting about FRET: A Detailed Look at Several FRET Approximations." Arizona State University, Department of Physics. 6 October 2010.

23. "Fretting about FRET: A Detailed Look at Several FRET Approximations." Valparaiso University, Department of Chemistry. 30 April 2010.

24. "Fretting about FRET: A Detailed Look at Several FRET Approximations." University of Pisa, Centre for Theoretical and Computational Chemistry. 9 April 2010.

25. "Fretting about FRET: A Detailed Look at Several FRET Approximations." Max Planck Institute, Göttingen, Germany, Department of Theoretical and Computational Biophysics. 6 April 2010.

26. "Fretting about FRET: Breakdown of the Ideal Dipole Approximation." University of Massachusetts, Physics Department.   February 2010.

27. "Fretting about FRET: Breakdown of the Ideal Dipole Approximation." American Chemical Society National Meeting, Salt Lake City, UT   23 March 2009.

28. "Getting to Know Molecules, One at a Time." Hope College, Department of Chemistry. 29 August 2008.

29. "Fretting about FRET: Using computers and lasers to re-examine the use of FRET as a spectroscopic ruler." University of Pittsburgh, Chemistry Department. 28 August 2008.

30. "Combining Fluorescence Spectroscopy and Computation to Examine Structural

Dynamics in Biological Systems." University of Southern California, Chemistry Department. 21 April 2008.

31. "Computational Analysis of the Assumptions Underlying Use of FRET as a Spectroscopic Ruler." Notre Dame University, Chemistry Department. 4 May 2006.

32. "Computational Analysis of the Assumptions Underlying Use of FRET as a Spectroscopic Ruler." Midwest Computational Structural Biology Workshop, Brook Lodge, Augusta, MI. 30 April 2005.

33. "Can physics and biology get along? Developing new tools in structural biology through spectroscopy and computation." Grand Valley State University, Chemistry Department. 8 April 2005.

34. "Developing a Hybrid Classical and Quantum Mechanical Model to Describe Solvation Dynamics." University of Florida, Quantum Theory Project. 26 January 2005.

35. "Can physics and biology get along? Using computation and spectroscopy to develop new tools in structural biology." Michigan State University, Chemistry Department. 21 July 2004.

36. "Developing a Hybrid Classical and Quantum Mechanical Model to Describe Solvation Dynamics or Why We Need Lots of CPUs." Hope College, Physics and Engineering Department. 20 February 2004.

37. "Can physics and biology get along? Using computation and spectroscopy to study regulation." Calvin College, Chemistry and Biochemistry Department. 4 December 2003.

38. "Can physics and biology get along? Using computation and spectroscopy to study regulation." Carthage College, Science Division Colloquium. 29 September 2003.

39. "Can physics and biology get along? Using computation and spectroscopy to study regulation." Andrews University, Chemistry Department. 27 March 2003.

40. "Reconciling Spectroscopy with Computation: from Photosynthetic Light-Harvesting to Regulatory Pathways." Wayne State University, Physical and Analytical Chemistry Seminar. 9 October 2002.

41. "How Can I Learn to Teach When All I do is Research? Preparing to Teach in a Research World." The University of Chicago, Lessons from New Faculty: Teaching Across the Physical Sciences Conference. 1 June 2002.

42. "Energy Transfer in Photosynthesis and Other Short Stories About Reconciling Non-Linear Spectroscopy with Computational Chemistry." Bowling Green University, The Center for Photochemical Sciences. 27 February 2002.

43. "Examining Phospholamban Binding Through Time-resolved Fluorescence and Computations." University of Minnesota, D. Thomas group meeting. 24 September 2001.

44. "Understanding Photosynthesis Through Non-linear Spectroscopy and Computations." University of Minnesota, Structural Biology Seminar. 24 September 2001.

45. "The Role of Carotenoids in Bacterial Light-Harvesting." Lund University, Villy Sundström group meeting. June 1999.

46. "The Role of Carotenoids in Bacterial Light-Harvesting." Tenth Annual Western Photosynthesis Conference. Asilomar. 6 January 1999.

47. "Echoes of Light: Non-linear Ultrafast Spectroscopy." Truman State University, Chemistry Department. 29 October 1998.

48. "Observing the First Steps in Photosynthesis by Time-Resolved Spectroscopy." Truman State University, Physics Department. 26 October 1998.

Contributed Presentations at National or International Meetings

49. "Recruiting And Retaining The Next Generation Of Stem Professionals – The Day1: Watershed Research Community At Hope College" Society for Freshwater Science Annual Meeting, Detroit, MI. 24 May 2018 (talk).

50. "Two tales of molecular dynamics parameters: Fluorescent protein chromophores and aqueous ions", 251st American Chemical Society National Meeting, San Diego, CA, 14 March 2016. (talk)

51. "Bringing molecular modeling into the high school classroom", American Chemical Society National Meeting, Dallas, TX. 20 March 2014. (talk)

52. "Modeling fluorescence observables, particularly for FRET experiments, using Markov chain analysis of molecular dynamics simulations", American Chemical Society National Meeting, Dallas, TX. 19 March 2014. (talk)

53. "Modeling Fluorescence Observables, Particularly for FRET Experiments, Using Markov Chain Analysis of Molecular Dynamics and Quantum Mechanics Simulations." 57th Annual Biophysical Society National Meeting. Philadelphia, PA. 6 February 2013. (poster)

54. "Modeling Fluorescence Observables, Particularly for FRET Experiments, Using Markov Chain Analysis of Molecular Dynamics and Quantum Mechanics Simulations." 56th Annual Biophysical Society National Meeting. San Diego, CA. 8 February 2012. (poster)

55. "Fretting About FRET: Examining the Underlying Assumptions." Graham R. Fleming Festschrift, University of California at Berkeley, Berkeley, CA. 15 July 2010. (poster)

56. "Fretting About FRET: Breakdown of the Ideal Dipole Approximation." 54th Annual Biophysical Society National Meeting, San Francisco, CA. 23 February 2010. (poster)

57. "Fretting About FRET." 52nd Annual Biophysical Society National Meeting, Long Beach, CA. 4 February 2008. (poster)

58. "Hybrid Molecular Dynamics-Quantum Mechanics Simulations of Condensed Phase Spectral Properties: Evaluation of Simulation Parameters." American Chemical Society National Meeting, Chicago, IL. 29 March 2007. (talk)

59. "Fretting about FRET: Correlation between κ and R." American Chemical Society

National Meeting, Chicago, IL. 27 March 2007. (talk)

60. "Hybrid molecular dynamics-quantum mechanics simulations of solvation dynamics." American Chemical Society National Meeting, San Diego, CA. 14 March 2005. (talk)

61. "Molecular Dynamics Studies of a Highly-Charged Peptide: A Possible Sequence-Function Relationship." American Chemical Society National Meeting, Washington D.C. 20-24 August 2000. (poster)

62. "Transient Absorption Studies of the Peridinin Chlorophyll-a Protein Light-Harvesting Complex." American Chemical Society National Meeting, Washington D.C. 20-24 August 2000. (poster)

63. "Dynamics Studies of a Stable Heptapeptide." Gordon Conference on Vibrational Spectroscopy. Salve Regina Unviersity. 7-10 Aug 2000. (poster)

64. "Molecular Dynamics Studies of a Stable Heptapeptide." Gordon Conference on Biopolymers. Salve Regina Unviersity. 19-22 June 2000. (poster)

65. "Fluorescence Upconversion and ab initio Studies of the Light-Harvesting Function of Carotenoids in Bacterial Light-Harvesting Antenna." 11th International Conference on Ultrafast Phenomena, Garmisch-Partenkirchen, Germany. 15 July 1998. (poster)

Presentations at National or International Meetings by Students and others (Presenters indicated with *)

66. C. Cooper*, I. DeLoach, A. Slater, R. Wade, S. Brokus, A.A Best, J. McMorris, B.P. Krueger, and M.J. Pikaart, "Interactions between chemical and environmental factors and bacterial community composition in a Great Lakes watershed", Experimental Biology, San Diego, CA, 5 April, 2020. (poster)

67. B. Fry*, D. Wade*, F. Fishman, J.W. Peterson, M.J. Pikaart, E. Schumann, J. Stid, J. Peterson, S. Brokus, R. Wade, A.A Best, and B.P. Krueger, "Heavy Metals in Water: A Global Survey to Characterize Untreated Drinking Sources", Annual Meeting of the Geological Society of America, Phoenix, AZ, 22 September, 2019. (poster)

68. C. Cooper*, C. Belica, A. Pearch, E. Schumann, S. Brokus, F. Moen, R. Wade, A.A Best, B.P. Krueger, and M.J. Pikaart, "Bacterial Community Composition and Environmental Factors in a Hypereutrophic Watershed", ASBMB Annual Meeting, Orlando, FL, 8 April, 2019. (poster)

69. M. Solórzano*, K.C. Franz, M.L. Luke, N.A. Ladd, E.A. Eaton, C.O. Da Silva, S.M. Degnan, M.M. Olesh, L.A. Chase, A.P. Putzke, and B.P. Krueger, "Investigating the Role of xCT in Neuroregeneration" Annual Biomedical Research Conference for Minority Students, Indianapolis, IN, 14 November 2018. (poster)

70. R. Wade*, S. Brokus, F. Moen, C. Payne, T. Garcia, C. Harders, A. Jeavons, M. Luke, A. Klein, A. Parshall, L. Perez, E. Plouch, A. Slater, D. Wade, B.P. Krueger, M.J. Pikaart, A.A. Best, "Environmental Factors Affecting Bacterial Community Composition In The Hypereutrophic Macatawa Watershed", Society for Freshwater Science Annual Meeting, Detroit, MI. 22 May 2018 (talk).

71. <u>E. Plouch</u>*, <u>A. Jeavons</u>, <u>M. Luke</u>, <u>A. Parshall</u>, <u>J. Spry</u>, <u>D. Wade</u>, S. Brokus, R. Wade, B.P. Krueger, M.J. Pikaart, A.A. Best, "Monitoring Nutrient Levels And Sediment In Macatawa Watershed", Society for Freshwater Science Annual Meeting, Detroit, MI. 23 May 2018 (poster).

72. <u>M. Solórzano</u>*, <u>N.A. Ladd</u>, <u>K.C. Franz</u>, <u>C.O. Da Silva</u>, L.A. Chase, A.P. Putzke, and B.P. Krueger, "Identifying the Expression Patterns of xCT in Zebrafish to Determine its Role in Neuroregeneration" Annual Biomedical Research Conference for Minority Students, Phoenix, AZ, 3 November 2017. (poster)

73. <u>M. Solórzano</u>*, <u>N.A. Ladd</u>, <u>K.C. Franz</u>, <u>C.O. Da Silva</u>, L.A. Chase, A.P. Putzke, and B.P. Krueger, "Identifying the Expression Patterns of xCT in Zebrafish to Determine its Role in Neuroregeneration" American Society for Biochemistry and Molecular Biology National Meeting, Chicago, IL, 25 April 2017. (poster)

74. <u>D.E. Clark</u>*, <u>J.C. Dood</u>, and B.P. Krueger, "Developing Monovalent Ion Parameters for the Optimal Point Charge (OPC) Water Model." American Society for Biochemistry and Molecular Biology National Meeting, Chicago, IL, 24 April 2017. (poster)

75. <u>N.A. Ladd</u>*, A.P. Putzke, L.A. Chase, and B.P. Krueger, "Interrogating the Role of xCT in Neuroregeneration through Laser Ablation of Zebrafish Neurons" 251st American Chemical Society National Meeting, BIOL Session, San Diego, CA, 15 March 2016 (poster).

76. <u>J.C. Dood</u>*, B.P. Krueger, "Developing monovalent ion parameters for the optimal point charge (OPC) water model", 251st American Chemical Society National Meeting, COMP Session, San Diego, CA, 15 March 2016 (poster).

77. <u>D.L. Blood</u>*, <u>A.M. Rosnik</u>, and B.P. Krueger, "Parameterizing fluorescent protein chromophores for molecular dynamics simulations", 251st American Chemical Society National Meeting, COMP Session, San Diego, CA, 15 March 2016 (poster).

78. <u>N.A. Ladd</u>*, A.P. Putzke, L.A. Chase, and B.P. Krueger, "Interrogating the Role of xCT in Neuroregeneration through Laser Ablation of Zebrafish Neurons" 250th American Chemical Society National Meeting, PHYS Session, Boston, MA, 19 August 2015 (poster). Won best PHYS poster.

79. <u>J.C. Dood</u>*, B.P. Krueger, "Developing monovalent ion parameters for the optimal point charge (OPC) water model" 250th American Chemical Society National Meeting, COMP Session, Boston, MA, 18 August 2015 (poster).

80. <u>J.C. Dood</u>*, B.P. Krueger, "Developing monovalent ion parameters for the optimal point charge (OPC) water model", 250th American Chemical Society National Meeting, SCI-MIX Session, Boston, MA, 17 August 2015 (poster).

81. M.E. Anderson*, B.P. Krueger, <u>A. Schuiling</u>, T. Gugino. "Determining the chemical formula of unknown crystals as a semester-long inquiry theme for general chemistry lab." Biennial Conference on Chemical Education, Grand Valley State University, Allendale, MI, August 2014. (talk)

82. <u>A.C. Cutshall</u>, <u>C.J. Davis</u>*, <u>T.C. Hoffman</u>*, <u>D.W. Summers</u>, and B.P. Krueger. "Single-

molecule florescence spectroscopy using a home-built microscope", American Chemical Society National Meeting, Dallas, TX. 17 March 2014. (poster)

83. C.J. Kimmel*, and B.P. Krueger*. "Introducing Molecular Modeling to High School Students and Teachers." ChemEd 2011 International Conference, Western Michigan University. 27 July 2011. (talk)

84. A.A. Cassabaum*, A.S. Ortega*, C.A. Gobrogge, C.J. Calyore, J.D. Lewis, D.A. Paul, A.L. Speelman, C.M. Tobert, and B.P. Krueger. "Investigating Biopolymer Functions and Probe Dynamics By Utilizing Fluorescent Techniques." 241st American Chemical Society National Meeting. Anaheim, CA. 27-31 March 2011. (poster)

85. A.L. Speelman*, A.S. Ortega, D.A. Paul, B.A. Leland, and B.P. Krueger. "Modeling Fluorescently Tagged DNA and RNA Oligonucleotides for Direct Comparison to FRET Experiments." 54th Biophysical Society Annual Meeting. San Francisco, CA. 23 February 2010. (poster)

86. A.S. Ortega*, A.L. Speelman, D.A. Paul, B.A. Leland, and B.P. Krueger. "Modeling Fluorescently Tagged DNA and RNA Oligonucleotides for Direct Comparison to Fluorescence-detected Resonance Energy Transfer (FRET) Experiments." 20th Annual Argonne Symposium for Undergraduates in Science, Engineering and Mathematics, Argonne National Laboratory, Argonne, IL. 13 October 2009 (talk)

87. J.D. Lewis*, D.A. Paul, D.P. Millar, M.J. Pikaart, and B.P. Krueger. "The Study of the Structural Dynamics and Binding of Biopolymers via the Use of Fluorescence-Detected Resonance Energy Transfer (FRET)." Council on Undergraduate Research Posters on the Hill, Washington, D. C. 5 May 2009. (poster)

88. D.A. Paul*, B.A. Leland, J.D. Lewis, and B.P. Krueger. "Bridging the Gap Between Computation and Experiment to Understand Structural Dynamics in the Hairpin Ribozyme." MERCURY Conference on Undergraduate Computational Chemistry, Hamilton College, Clinton, NY. 4 August 2008. (poster)

89. J.D. Lewis*, D.A. Paul, D.P. Millar, M.J. Pikaart, and B.P. Krueger. "The Study of the Structural Dynamics and Binding of Biopolymers via the Use of Fluorescence-Detected Resonance Energy Transfer (FRET)." Tenth Annual Beckman Scholars Symposium, Irvine, CA. 25 July 2008. (poster)

90. J.D. Lewis*, L.R. Hartsell, N.E. Kuiper, C.M. Tobert, M.J. Pikaart, and B.P. Krueger. "The Study of the Structural Dynamics and Binding of Biopolymers via the Use of Fluorescence-Detected Resonance Energy Transfer (FRET)." Biophysical Society National Meeting, Long Beach, CA. 6 February 2008. (poster)

91. L.R. Harsell*, A.J. Huisman, B.P. Krueger, and M.J. Pikaart. "Thermodynamic exploration of eosin-lysozyme binding: A physical chemistry and biochemistry laboratory experiment." American Chemical Society National Meeting, Chicago, IL. 26 March 2007. (poster)

92. K.L. Hinkle* and B.P. Krueger. "Analysis of domain flexibility in fluorescently tagged fusion proteins using molecular dynamics simulations." American Chemical Society National Meeting, Atlanta, GA. 27 March 2006. (poster)

93. D.B. VanBeek*, M.C. Zwier, C.J. Goltz, T.R. Stowe, B.L. Mason, and B.P. Krueger. "Development of a combined molecular dynamics (MD) and fluorescence-detected resonance energy transfer (FRET) method for structural biology." National Beckman Scholars Meeting, Irvine, CA. 28-30 July 2005. (poster)

94. D.B. VanBeek*, M.C. Zwier, C.J. Goltz, T.R. Stowe, B.L. Mason, and B.P. Krueger. "Development of a combined molecular dynamics (MD) and fluorescence-detected resonance energy transfer (FRET) method for structural biology." Biophysical Society National Meeting, Long Beach, CA. 13 February 2005. (poster)

95. J.M. Shorb*, M.E. Silver, and B.P. Krueger. "Modeling the Behavior of Siloxane Polymers as Emulsifiers using Molecular Dynamics Simulations." 37th Silicone Symposium, University of Pennsylvania. 19-21 May 2004. (poster)

96. T.R. Stowe*, D.B. VanBeek, M.C. Zwier, C.J. Goltz, S. DeLange, B.L. Mason, and B.P. Krueger. "Development of a combined molecular dynamics (MD) and fluorescence-detected resonance energy transfer (FRET) method for structural biology." Biophysical Society National Meeting, Washington, DC. 15 February 2004. (poster)

97. D.B. VanBeek*, T.R. Stowe, M.C. Zwier, C.J. Goltz, S. DeLange, B.L. Mason, and B.P. Krueger. "Development of a combined molecular dynamics (MD) and fluorescence-detected resonance energy transfer (FRET) method for structural biology." American Association for the Advancement of Science National Meeting, Seattle, WA. 12-13 February 2004. (poster)

98. C.J. Goltz*, B.L. Mason*, J.L. Broyles, M.A. Burnatowska-Hledin, and B.P. Krueger. "Use of Steady-State and Time-Resolved Fluorescence To Characterize Vasopressin-Receptor Binding." Biophysical Society National Meeting, San Antonio, TX. 1-5 March 2003. (poster)

99. M.C. Zwier* and B.P Krueger. "Use of Molecular Dynamics Simulations in Analysis of Fluorescence-Detected Resonance Energy Transfer (FRET) Experiments." Biophysical Society National Meeting, San Antonio, TX. 1-5 March 2003. (poster)

Presentations at Regional Meetings by Students, Postdocs, or Staff Under My Supervision

1. C. Cooper*, J. McMorris, A. Slater, R. Wade, S. Brokus, A.A Best, B.P. Krueger, and M.J. Pikaart, "Interactions between chemical and environmental factors and bacterial community composition in a Great Lakes watershed", Midstates Consortium for Math and Science Undergraduate Research Symposium in Biological Science and Psychology. The University of Chicago (online), 31 October, 2020. (talk)

2. A.J. Bauer*, M. G. Rabitoy*, Aaron A. Best, and B.P. Krueger, "Using Machine Learning to Identify Sources of Bacteria in Water" Thirty-fifth Midwest Undergraduate Computational Chemistry Consortium Conference. Online due to COVID, 29 July 2020. (poster)

3. K.L. Breyfogle*, D.L. Blood, A.M. Rosnik, and B.P. Krueger, "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations" Thirty-fourth

Midwest Undergraduate Computational Chemistry Consortium Conference. Online, 4 February 2020. (poster)

4. <u>M. G. Rabitoy*</u>, <u>A.J. Bauer*</u>, Aaron A. Best, and B.P. Krueger, "Using Machine Learning to Identify Sources of Bacteria in Water" Thirty-fourth Midwest Undergraduate Computational Chemistry Consortium Conference. Online, 4 February 2020. (poster)

5. <u>K.L. Breyfogle*</u>, <u>D.L. Blood</u>, <u>A.M. Rosnik</u>, and B.P. Krueger, "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations" Thirty-third Midwest Undergraduate Computational Chemistry Consortium Conference. The Ohio State University, 19 July 2019. (poster)

6. <u>M. G. Rabitoy*</u>, <u>A.J. Bauer*</u>, Aaron A. Best, and B.P. Krueger, "Using Machine Learning to Identify Sources of Bacteria in Water" Thirty-third Midwest Undergraduate Computational Chemistry Consortium Conference. The Ohio State University, 19 July 2019. (talk)

7. <u>A R. Prins*</u>, <u>Z. Snoek*</u>, and B.P. Krueger, "The Next Generation of High Performance Computing Using Containerization" Thirty-third Midwest Undergraduate Computational Chemistry Consortium Conference. The Ohio State University, 19 July 2019. (talk)

8. <u>K.L. Breyfogle*</u>, <u>D.L. Blood</u>, <u>A.M. Rosnik</u>, and B.P. Krueger, "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations" Thirty-second Midwest Undergraduate Computational Chemistry Consortium Conference. Online, 7 February 2019. (poster)

9. <u>A R. Prins*</u>, <u>Z. Snoek*</u>, and B.P. Krueger, "The Next Generation of High Performance Computing Using Containerization" Thirty-second Midwest Undergraduate Computational Chemistry Consortium Conference. Online, 7 February 2019. (poster)

10. <u>K.L. Breyfogle*</u>, <u>D.L. Blood</u>, <u>A.M. Rosnik</u>, and B.P. Krueger, "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations" Midstates Consortium for Math and Science Undergraduate Research Symposium in Biological Science and Psychology. The University of Chicago, 3 November 2018. (talk)

11. <u>E.A. Eaton*</u>, <u>M. Solórzano</u>, <u>K.C. Franz</u>, <u>M.L. Luke</u>, <u>N.A. Ladd</u>, <u>C.O. Da Silva</u>, <u>S.M. Degnan</u>, <u>M.M. Olesh</u>, L.A. Chase, A.P. Putzke, and B.P. Krueger, "Investigating the Role of xCT in Neuroregeneration" Midstates Consortium for Math and Science Undergraduate Research Symposium in Biological Science and Psychology. The University of Chicago, 3 November 2018. (poster)

12. <u>A R. Prins*</u>, <u>Z. Snoek*</u>, and B.P. Krueger, "The Next Generation of High Performance Computing Using Containerization" Thirty-first Midwest Undergraduate Computational Chemistry Consortium Conference. University of Minnesota, 23 July 2018. (talk)

13. <u>K L. Breyfogle*</u>, <u>D.L. Blood</u>, <u>A.M. Rosnik</u>, and B.P. Krueger, "Developing MD Parameters for Fluorescent Proteins" Thirty-first Midwest Undergraduate Computational Chemistry Consortium Conference. University of Minnesota, 23 July 2018. (talk)

14. <u>Leah Krudy*</u>, Dane Morgan, and B.P. Krueger, "Using Neural Nets/Machine Learning to Analyze Radiation Damage in Steel" Thirty-first Midwest Undergraduate Computational Chemistry Consortium Conference. University of Minnesota, 23 July 2018. (talk)

15. <u>A R. Prins*</u>, <u>Z. Snoek*</u>, and B.P. Krueger, "The Next Generation of High Performance Computing Using Containerization" Thirtieth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 31 January 2018. (poster)

16. <u>D.E. Clark*</u>, <u>J.C. Dood</u>, and B.P. Krueger, "Developing monovalent ion parameters for the Optimal Point Charge (OPC) water model" Thirtieth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 31 January 2018. (poster)

17. <u>D.E. Clark*</u>, <u>J.C. Dood</u>, and B.P. Krueger, "Developing monovalent ion parameters for the Optimal Point Charge (OPC) water model" Twenty-ninth Midwest Undergraduate Computational Chemistry Consortium Conference. University of Illinois. 1 August 2017. (talk)

18. <u>A R. Prins*</u>, <u>Z. Snoek*</u>, and B.P. Krueger, "The Next Generation of High Performance Computing Using Containerization" Twenty-ninth Midwest Undergraduate Computational Chemistry Consortium Conference. University of Illinois. 1 August 2017. (talk)

19. <u>D.E. Clark*</u>, <u>J.C. Dood</u>, and B.P. Krueger, "Developing monovalent ion parameters for the Optimal Point Charge (OPC) water model" Twenty-eighth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 9 February 2017. (poster)

20. <u>D.E. Clark*</u>, <u>J.C. Dood</u>, and B.P. Krueger, "Developing monovalent ion parameters for the Optimal Point Charge (OPC) water model" Midstates Consortium for Math and Science Undergraduate Research Symposium in the Physical Sciences, Mathematics, and Computer Science, Washington University, 4-5 November 2016. (poster)

21. <u>M. Solórzano*</u>, <u>N.A. Ladd</u>, <u>K.C. Franz</u>, <u>C.O. Da Silva</u>, L.A. Chase, A.P. Putzke, and B.P. Krueger, "Identifying the Expression Patterns of xCT in Zebrafish to Determine its Role in Neuroregeneration" Midstates Consortium for Math and Science Undergraduate Research Symposium Biology and Psychology Symposium, Washington University, 4-5 November 2016. (poster)

22. <u>D.E. Clark*</u>, <u>J.C. Dood</u>, and B.P. Krueger, "Developing Ion Parameters for the Optimal Point Charge (OPC) Water Model." Twenty-Seventh Midwest Undergraduate Computational Chemistry Consortium Conference. University of Wisconsin, Madison, WI. 21 July 2016. (talk)

23. <u>D.L. Blood*</u>, <u>A.M. Rosnik</u>, and B.P. Krueger, "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations." Twenty-sixth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 3 February 2016. (poster)

24. <u>A.M. Muñoz*</u>, <u>L.E. Messer</u>, <u>A.R. Prins</u>, B.P. Krueger, and J.G. Gillmore. "DFT calculations of bond lengths and bond orders to examine differential ring opening in quinazolinespirohexadienones." Twenty-sixth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 3 February 2016. (poster)

25. A.R. Prins*, A.M. Muñoz, A.J. Prins, B.P. Krueger, and J.G. Gillmore. "Computational modeling of the thermodynamics of proposed reactions of N,N-dimethylaniline with BX₃." Twenty-sixth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 3 February 2016. (poster)

26. J.C. Dood* and B.P. Krueger, "Developing Monovalent Ion Parameters for the Optimal Point Charge (OPC) Water Model." Twenty-sixth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 3 February 2016. (poster)

27. N.A. Ladd*, A.P. Putzke, L.A. Chase, and B.P. Krueger, "Interrogating the Role of xCT in Neuroregeneration through Laser Ablation of Zebrafish Neurons" Midstates Consortium for Math and Science Undergraduate Research Symposium Biology and Psychology Symposium, Washington University, 6-7 November 2015. (talk)

28. J.C. Dood* and B.P. Krueger, "Developing Ion Parameters for the Optimal Point Charge (OPC) Water Model." Midstates Consortium for Math and Science Undergraduate Research Symposium Physical Sciences, Mathematics, and Computer Science Symposium, University of Chicago, 13-14 November 2015. (talk)

29. D.L. Blood*, A.M. Rosnik, and B.P. Krueger, "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations." Midstates Consortium for Math and Science Undergraduate Research Symposium Physical Sciences, Mathematics, and Computer Science Symposium, University of Chicago, 13-14 November 2015. (poster)

30. J.C. Dood* and B.P. Krueger, "Developing Ion Parameters for the Optimal Point Charge (OPC) Water Model." Twenty-Fifth Midwest Undergraduate Computational Chemistry Consortium Conference. Northwestern University, Evanston, IL. 23 July 2015. (talk)

31. D.L. Blood*, A.M. Rosnik, and B.P. Krueger, "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations." Twenty-Fifth Midwest Undergraduate Computational Chemistry Consortium Conference. Northwestern University, Evanston, IL. 23 July 2015. (talk)

32. N.A. Ladd*, D. Fernandez*, A.P. Putzke, L.A. Chase, and B.P. Krueger, "Structural Modeling of the Endocytic Motifs in the Carboxy Terminus of xCT" Twenty-Fifth Midwest Undergraduate Computational Chemistry Consortium Conference. Northwestern University, Evanston, IL 24 July 2015. (poster)

33. A.M. Muñoz*, L.E. Messer, Anna R. Prins, B.P. Krueger, and J.G. Gillmore "DFT calculations of bond lengths and bond orders to examine differential ring opening in quinazolinespirohexadienones." Twenty-Fifth Midwest Undergraduate Computational Chemistry Consortium Conference. Northwestern University, Evanston, IL 24 July 2015. (poster)

34. Anna R. Prins*, A.M. Muñoz, Amber J. Prins, B.P. Krueger, and J.G. Gillmore, "Computational Modeling of the Thermodynamics of Proposed Reactions of N,N-Dimethylaniline with BX3." Twenty-Fifth Midwest Undergraduate Computational Chemistry Consortium Conference. Northwestern University, Evanston, IL 24 July 2015. (poster)

35. J.C. Dood* and B.P. Krueger, "Developing Ion Parameters Using Shared GPU

Accelerator Hardware." Twenty-Fourth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 17 February 2015. (poster)

36. D.L. Blood*, A.M. Rosnik, and B.P. Krueger, "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations." Twenty-Fourth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 17 February 2015. (poster)

37. N.A. Ladd*, L.A. Chase, A.P. Putzke, and B.P. Krueger, "Exploring the Role of xCT in Neuroregeneration through Laser Ablation of Zebrafish Neurons" Midstates Consortium for Math and Science Undergraduate Research Symposium in the Biophysical Sciences and Psychology, The University of Chicago, 7-8 November 2014. (talk)

38. N.A. Ladd*, L.A. Chase, A.P. Putzke, and B.P. Krueger, "Exploring the Role of xCT in Neuroregeneration through Laser Ablation of Zebrafish Neurons" Midwestern Symposium on Undergraduate Research in Chemistry, Michigan State University, East Lansing, MI, 11 October 2014. (poster)

39. J. C. Dood* and B.P. Krueger "Developing Ion Parameters Using Shared GPU Accelerator Hardware" Midwestern Symposium on Undergraduate Research in Chemistry, Michigan State University, East Lansing, MI, 11 October 2014. (poster)

40. J.C. Dood* and B.P. Krueger. "Developing Ion Parameters Using Shared GPU Accelerator Hardware", Twenty-Third Midwest Undergraduate Computational Chemistry Consortium Conference. Iowa State University, Ames, IA. 28 Jul 2014. (talk)

41. D. Blood*, A.M. Rosnik, and B.P. Krueger. "Parameterizing Fluorescent Protein Chromophores for Molecular Dynamics Simulations", Twenty-Third Midwest Undergraduate Computational Chemistry Consortium Conference. Iowa State University, Ames, IA. 28 Jul 2014. (talk)

42. C. Dummer*, S. Ipri-Brown, C.L. Ellis, C.J. Kimmel, and B.P. Krueger. "STEM Inquiry Curriculum/Equipment Lending Library at Hope College CSI." Michigan Science Teachers Association Meeting, Lansing, MI. 7 March 2014. (talk)

43. C.J. Davis*, A.C. Cutshall, T.C. Hoffman, D.W. Summers, A.S. Ortega, and B.P. Krueger, "Home-Built Single-molecule Fluorescence Spectroscopy", Midstates Consortium for Math and Science, 2013 Undergraduate Research Symposium in the Physical Sciences, Math, and Computer Science, The University of Chicago, Chicago, IL. 25-26 October 2013. (poster)

44. C. Dummer*, C.L. Ellis, C.J. Kimmel, and B.P. Krueger. "Molecular Modeling: A Computational Science & Modeling Approach." Michigan Science Teachers Association Meeting, Eastern Michigan University, Ypsilanti, MI. 9 March 2013. (talk)

45. A.E. Cook*, A.M. Stevenson*, D.W. Summers, A.A. Cassabaum, C.A. Gobrogge, A.L. Speelman, D.A. Paul, B.A. Leland, A.S. Ortega, B.P. Krueger. "Extending the AMBER Force Field to Describe Fluorescent Probes." Twentieth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 5 February 2013. (poster)

46. A.C. Cutshall*, C.J. Davis*, D.W. Summers*, and B.P. Krueger. "Bridging Single-Molecule Spectroscopy and Molecular Dynamics Simulations." Nineteenth Midwest Undergraduate Computational Chemistry Consortium Conference, University of Minnesota, Minneapolis, MN. 16 July 2012. (talk)

47. A.E. Cook*, A.A. Cassabaum, C.A. Gobrogge, A.S. Ortega, A.M. Stevenson, C.J. Calyore, J.D. Lewis, D.A. Paul, A.L. Speelman, C.M. Tobert, and B.P. Krueger. "Investigating Biopolymer Functions and Probe Dynamics By Utilizing Fluorescent Techniques." West Michigan Regional Undergraduate Science Research Conference, Van Andel Research Institute, Grand Rapids, MI. 12 November 2011. (poster)

48. C.J. Kimmel*, C.L. Ellis, and B.P. Krueger. "Introducing Inquiry-Based Computational Science and Modeling to High School Students and Teachers." 17th Midwest Undergraduate Computational Chemistry Consortium Conference. The University of Chicago, Chicago, IL. 25-26 July 2011. (poster)

49. A.E. Cook*, D.W. Summers*, A.S. Ortega*, A.M. Stevenson, A.A. Cassabaum, C.A. Gobrogge, A.L. Speelman, D.A. Paul, B.A. Leland, B.P. Krueger. "Extending the AMBER Force Field to Describe Fluorescent Probes." 17th Midwest Undergraduate Computational Chemistry Consortium Conference. The University of Chicago, Chicago, IL. 25-26 July 2011. (talk)

50. C.L. Ellis* and B.P. Krueger. "Web What?! Easy 3D Chemistry Tools for High School Students." Michigan Science Teachers Association 57th Annual Conference. Lansing, MI. 25-26 February 2011. (talk)

51. C.L. Ellis* and B.P. Krueger. "Web What?! Easy 3D Chemistry Tools for High School Students." Michigan Space Grant Consortium Meeting. Ann Arbor, MI. 13 November 2010. (talk)

52. A.S. Ortega*, A.A. Cassabaum, C.A. Gobrogge, A.E. Cook, A.M. Stevenson, C.J. Calyore, J.D. Lewis, D.A. Paul, A.L. Speelman, C.M. Tobert, and B.P. Krueger. "Investigating Biopolymer Functions and Probe Dynamics By Utilizing Fluorescent Techniques." Midstates Consortium for Math and Science, 2010 Undergraduate Research Symposium – Physical Sciences, Mathematics and Computer Science, Washington University, St. Louis, MO. 12-14 November 2010. (poster)

53. A.A. Cassabaum*, C.A. Gobrogge*, A.E. Cook*, A.M. Stevenson*, A.S. Ortega, C.J. Calyore, J.D. Lewis, D.A. Paul, A.L. Speelman, C.M. Tobert, and B.P. Krueger. "Investigating Biopolymer Functions and Probe Dynamics By Utilizing Fluorescent Techniques." Midstates Consortium for Math and Science, 2010 Undergraduate Research Symposium – Biological Sciences and Psychology, Chicago, IL. 5-7 November 2010. (poster)

54. C.L. Ellis* and B.P. Krueger. "Introducing Inquiry-Based Computational Science and Modeling to High School Students and Teachers." Regional NSF-REU Summer Symposium. Holland, MI. 30 July 2010. (poster)

55. A.A. Cassabaum*, C.A. Gobrogge*, A.S. Ortega*, C.J. Calyore, J.D. Lewis, D.A. Paul, A.L. Speelman, C.M. Tobert, and B.P. Krueger. "Investigating Biopolymer Functions and Probe Dynamics By Utilizing Fluorescent Techniques." Regional NSF-REU

Summer Symposium. Holland, MI. 30 July 2010. (poster)

56. <u>C.L. Ellis*</u> and B.P. Krueger. "Web What?! Easy 3D Chemistry Tools for High School Students." Michigan Science Teachers Association 57th Annual Conference. Lansing, MI. 4-6 March 2010. (talk)

57. <u>A.L. Speelman*</u>, <u>D.A. Paul</u>, <u>B.A. Leland</u>, and B.P. Krueger. "Modeling Fluorescently Tagged DNA and RNA Oligonucleotides for Direct Comparison to Fluorescence-detected Resonance Energy Transfer (FRET) Experiments." 14th Midwest Undergraduate Computational Chemistry Consortium Symposium, Online. 9 February 2010. (poster)

58. <u>C.L. Ellis*</u> and B.P. Krueger. "Introducing Inquiry-based Computational Science and Modeling to High School Students and Teachers." Hope College Chemistry Department Seminar, Holland, MI. 15 January 2010. (talk)

59. <u>C.M. Tobert*</u>, <u>C.J. Calyore*</u>, <u>L.R. Hartsell</u>, <u>N.E. Kuiper</u>, <u>J.D. Lewis</u>, and B.P. Krueger. "Utilizing Fluorescent Techniques to Investigate Biopolymer Functions and Probe Dynamics." Third Annual West Michigan Regional Undergraduate Science Research Conference, Van Andel Research Institute, Grand Rapids, MI. 31 October 2009 (poster)

60. <u>A.S. Ortega*</u>, <u>A.L. Speelman</u>, <u>D.A. Paul</u>, <u>B.A. Leland</u>, and B.P. Krueger. "Modeling Fluorescently Tagged DNA and RNA Oligonucleotides for Direct Comparison to Fluorescence-detected Resonance Energy Transfer (FRET) Experiments." Midstates Consortium for Math and Science, 2009 Undergraduate Research Symposia in the Physical Sciences, Mathematics, and Computer Science, The University of Chicago, Chicago, IL. 4-6 November 2009. (poster)

61. <u>A.S. Ortega*</u>, <u>A.L. Speelman</u>, <u>D.A. Paul</u>, <u>B.A. Leland</u>, and B.P. Krueger. "Modeling Fluorescently Tagged DNA and RNA Oligonucleotides for Direct Comparison to Fluorescence-detected Resonance Energy Transfer (FRET) Experiments." Third Annual West Michigan Regional Undergraduate Science Research Conference, Van Andel Research Institute, Grand Rapids, MI. 31 October 2009   (poster)

62. <u>C.L. Ellis*</u> and B.P. Krueger. "Introducing Inquiry-based Computational Science and Modeling to High School Teachers." Regional REU Summer Symposium, Notre Dame University, South Bend, IN. 31 July 2009. (poster)

63. <u>A.S. Ortega*</u>, <u>A.L. Speelman</u>, <u>D.A. Paul</u>, <u>B.A. Leland</u>, and B.P. Krueger. "Modeling Fluorescently Tagged DNA and RNA Oligonucleotides for Direct Comparison to Fluorescence-detected Resonance Energy Transfer (FRET) Experiments." 13th Midwest Undergraduate Computational Chemistry Consortium Symposium, Northwestern University, Evanston, IL. 26-29 July 2009. (poster)

64. <u>C.M. Tobert*</u>, <u>L.R. Hartsell</u>, <u>N.E. Kuiper</u>, <u>J.D. Lewis</u>, and B.P. Krueger. "Utilizing Fluorescence Techniques to Investigate Biopolymer Function and Probe Dynamics." 13th Midwest Undergraduate Computational Chemistry Consortium Symposium, Northwestern University, Evanston, IL. 26-29 July 2009. (poster)

65. <u>A.L. Speelman*</u>, <u>D.A. Paul</u>, <u>B.A. Leland</u>, and B.P. Krueger. "Modeling Fluorescently Tagged DNA and RNA Oligonucleotides for Direct Comparison to FRET

Experiments." 13th Midwest Undergraduate Computational Chemistry Consortium Symposium, Northwestern University, Evanston, IL. 26-29 July 2009. (talk)

66. C.L. Ellis* and B.P. Krueger. "Introducing Inquiry-based Computational Science and Modeling to High School Teachers." 13th Midwest Undergraduate Computational Chemistry Consortium Symposium, Northwestern University, Evanston, IL. 26-29 July 2009. (talk)

67. D.A. Paul*, B.A. Leland, and B.P. Krueger. "Bridging the Gap Between Computation and Experiment to Understand Structural Dynamics in the Hairpin Ribozyme." Midstates Science and Mathematics Consortium, Twelth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 4 February 2009. (poster)

68. C.M. Tobert*, L.R. Hartsell, N.E. Kuiper, J.D. Lewis, B.P. Krueger and M.J. Pikaart. "Utilizing fluorescence anisotropy to better understand the binding affinity of the GATA/1 complex." Midstates Science and Mathematics Consortium, 2008 Undergraduate Research Symposia in the Biological Sciences and Psychology, Chicago, IL. 1 November 2008. (poster)

69. D.A. Paul*, B.A. Leland, and B.P. Krueger. "Bridging the Gap Between Computation and Experiment to Understand Structural Dynamics in the Hairpin Ribozyme." Midstates Science and Mathematics Consortium, 2008 Undergraduate Research Symposia in the Biological Sciences and Psychology, Chicago, IL. 1 November 2008. (poster)

70. J.D. Lewis*, L.R. Hartsell, N.E. Kuiper, and B.P. Krueger. "The Study of the Structural Dynamics and Binding of Biopolymers via the Use of Fluorescence-Detected Resonance Energy Transfer (FRET)." 2nd Annual West Michigan Regional Undergraduate Science Research Conference, Grand Rapids, MI. 1 November, 2008. (poster)

71. D.A. Paul*, B.A. Leland, and B.P. Krueger. "Bridging the Gap Between Computation and Experiment to Understand Structural Dynamics in the Hairpin Ribozyme." 7th annual MERCURY conference, Hamilton College, Clinton, NY. July 2008. (poster)

72. D.A. Paul*, B.A. Leland, and B.P. Krueger. "Bridging the Gap Between Computation and Experiment to Understand Structural Dynamics in the Hairpin Ribozyme." Tenth Midwest Undergraduate Computational Chemistry Consortium Conference. Online. 4 March 2008. (poster)

73. L.R. Hartsell, N.E. Kuiper, J.D. Lewis, C.M. Tobert*, B.P. Krueger, and M.J. Pikaart. "Utilizing Fluorescence Spectroscopy and Computation to Better Understand Protein/DNA Interactions." Pew Midstates Science and Mathematics Consortium Undergraduate Research Symposium in the Physical Sciences and Mathematics, The University of Chicago. 9-11 November 2007. (poster)

74. L.R. Hartsell*, N.E. Kuiper, J.D. Lewis, C.M. Tobert*, B.P. Krueger, and M.J. Pikaart. "Utilizing Fluorescence Spectroscopy and Computation to Better Understand Protein/DNA Interactions." West Michigan Regional Undergraduate Science Research Conference, Van Andel Research Institute. 20 October 2007. (poster)

75. D.A. Paul*, B.A. Leland, and B.P. Krueger. "Bridging the Gap Between Computation

and Experiment to Understand Structural Dynamics in the Hairpin Ribozyme." West Michigan Regional Undergraduate Science Research Conference, Van Andel Research Institute. 20 October 2007. (poster)

76. D.A. Paul*, B.A. Leland*, and B.P. Krueger. "Bridging the Gap Between Computation and Experiments to Understand Structural Dynamics in the Hairpin Ribozyme." Ninth Midwest Undergraduate Computational Chemistry Conference, University of Illinois, Champagne-Urbana, IL. 30 July - 1 August, 2007. (talk)

77. L.R. Hartsell* and B.P. Krueger. "Evaluating Coulombic Coupling: How close is too close?" Ninth Midwest Undergraduate Computational Chemistry Conference, University of Illinois, Champagne-Urbana, IL. 30 July - 1 August, 2007. (talk)

78. J. Fredenburg and B.P. Krueger. "Using WebMO in Chemistry." Michigan Science Teachers Association Meeting, Amway Grand Hotel, Grand Rapids, MI. 16 March 2007. (workshop)

79. J.D. Lewis*, L.R. Hartsell, N.E. Kuiper, B.P. Krueger, and M.J. Pikaart. "Utilizing Steady-State and Time-Resolved Fluorescence to Probe DNA/Gata Binding Interactions." Pew Midstates Science and Mathematics Consortium Undergraduate Research Symposium in the Physical Sciences and Mathematics, The University of Chicago, Chicago, IL. 3-5 November 2006. (poster)

80. J.D. Lewis*, L.R. Hartsell, N.E. Kuiper*, B.P. Krueger, and M.J. Pikaart. "Utilizing Steady-State and Time-Resolved Fluorescence to Probe DNA/Gata Binding Interactions." Regional REU Symposium, Notre Dame University, South Bend, IN. 4 August 2006.

81. K.L. Hinkle* and B.P. Krueger. "Parameterization for DNA-Fluorophore Molecular Dynamics: My Blue/Green Period." Seventh Midwest Undergraduate Computational Chemistry Conference, Iowa State University, Ames, IA. 1 August, 2006. (talk)

82. C.M. Meeusen*, M.C. Zwier, J.M. Shorb, and B.P. Krueger. "A Hybrid Molecular Dynamics and Quantum Mechanics Method for Simulating Solvation Dynamics." Sixth Midwest Undergraduate Computational Chemistry Conference. Online. 6-10 February 2006.   (poster)

83. D.B. VanBeek*, M.C. Zwier, J.M. Shorb, and B.P. Krueger. "Development of a combined molecular dynamics (MD) and fluorescence-detected resonance energy transfer (FRET) method for structural biology." Sixth Midwest Undergraduate Computational Chemistry Conference. Online. 6-10 February 2006. (poster)

84. K.L. Hinkle* and B.P. Krueger. "Analysis of Domain Flexibility in Fluorescently Tagged Fusion Proteins Using Molecular Dynamics Simulations." Sixth Midwest Undergraduate Computational Chemistry Conference. Online. 6-10 February 2006. (poster)

85. K.L. Hinkle* and B.P. Krueger. "Analysis of Domain Flexibility in Fluorescently Tagged Fusion Proteins Using Molecular Dynamics Simulations." Fifth Midwest Undergraduate Computational Chemistry Conference, Minneapolis, MN. 11-13 July 2005. (talk)

86. D.B. VanBeek*, M.C. Zwier, J.M. Shorb, and B.P. Krueger. "Development of a combined molecular dynamics (MD) and fluorescence-detected resonance energy transfer (FRET) method for structural biology." Fifth Midwest Undergraduate Computational Chemistry Conference, Minneapolis, MN.
11-13 July 2005. (talk)

87. C.M. Meeusen*, M.C. Zwier, J.M. Shorb, and B.P. Krueger. "Molecular Dynamics and Quantum Mechanics Simulations of Solvation Dynamics." Fourth Midwest Undergraduate Computational Chemistry Conference. Online. 7-11 February 2005. (poster)

88. D.B. VanBeek*, M.C. Zwier, J.M. Shorb, and B.P. Krueger. "Development of a combined molecular dynamics (MD) and fluorescence-detected resonance energy transfer (FRET) method for structural biology." Fourth Midwest Undergraduate Computational Chemistry Conference. Online. 7-11 February 2005. (poster)

89. K.L. Hinkle* and B.P. Krueger. "Analysis of Domain Flexibility in Fluorescently Tagged Fusion Proteins Using Molecular Dynamics Simulations." Fourth Midwest Undergraduate Computational Chemistry Conference. Online. 7-11 February 2005. (poster)

90. C.M. Meeusen*, M.C. Zwier, J.M. Shorb, and B.P. Krueger. "Molecular Dynamics and Quantum Mechanics Simulations of Solvation Dynamics." Third Midwest Undergraduate Computational Chemistry Conference. Madison WI.
3-4 August 2004. (talk)

91. D.B. VanBeek*, M.C. Zwier, J.M. Shorb, and B.P. Krueger. "Development of a Combined Molecular Dynamics (MD) and Fluorescence-detected Resonance Energy Transfer (FRET) Method for Structural Biology." Third Midwest Undergraduate Computational Chemistry Conference, Madison WI. 3-4 August 2004. (talk)

92. J.M. Shorb*, B.P. Krueger, and M.E. Silver. "Modeling the Behavior of Siloxane Polymers as Emulsifiers using Molecular Dynamics Simulations." Second Midwest Undergraduate Computational Chemistry Conference. Online. 23-26 February 2004. (poster)

93. M.C. Zwier*, J.M. Shorb*, and B.P. Krueger. "Hybrid Molecular Dynamics-Quantum Mechanics Simulations of Solvation Dynamics." Second Midwest Undergraduate Computational Chemistry Conference. Online. 23-26 February 2004. (poster)

94. J.M. Shorb*, B.P. Krueger, and M.E. Silver. "Modeling the Behavior of Siloxane Polymers as Emulsifiers using Molecular Dynamics Simulations." Western Michigan Regional American Chemical Society Undergraduate Poster Competition, Grand Valley State University. 25 February 2004. (poster)

95. D.B. VanBeek*, M.C. Zwier, J.M. Shorb, and B.P. Krueger. "Development of a combined molecular dynamics (MD) and fluorescence-detected resonance energy transfer (FRET) method for structural biology." Western Michigan Regional American Chemical Society Undergraduate Poster Competition, Grand Valley State University. 25 February 2004. (poster)

96. M.C. Zwier*, J.M. Shorb, and B.P. Krueger. "Hybrid Molecular Dynamics-Quantum

Mechanics Simulations of Solvation Dynamics." Western Michigan Regional American Chemical Society Undergraduate Poster Competition, Grand Valley State University. 25 February 2004. (poster)

97. <u>D.B. VanBeek*</u> and B.P. Krueger. "Expression of chicken lysozyme in *E. coli* for development of a new fluorescence technique in structural biology." Pew Midstates Science and Mathematics Consortium Undergraduate Research Symposium in the Physical Sciences and Mathematics, The University of Chicago. 14-16 November 2003. (poster)

98. <u>M.C. Zwier*</u>, <u>J.M. Shorb</u>, and B.P. Krueger. "Hybrid molecular dynamics-quantum mechanics simulations of solvation dynamics." First Midwest Undergraduate Computational Chemistry Conference, Chicago, IL. 15-16 August 2003. (talk)

99. <u>J.M. Shorb*</u>, B.P. Krueger, and M.E. Silver. "Utilization of a Genetic Algorithm in the Development of Parameters for Modeling Siloxanes." 9th annual Electronic Computational Chemistry Conference. 1-31 March 2003. (poster)

100. <u>M.C. Zwier*</u>, <u>J.M. Shorb</u>, and B.P. Krueger. "Use of Molecular Dynamics Simulations in Analysis of Fluorescence-Detected Resonance Energy Transfer (FRET) Experiments." 9th annual Electronic Computational Chemistry Conference. 1-31 March 2003. (poster)

101. <u>C.J. Goltz*</u>, <u>B.L. Mason*</u>, and B.P. Krueger. "Fluorescence-Detected Resonance Energy Transfer (FRET) Studies using Time Correlated Single Photon Counting (TCSPC)." Pew mid-states undergraduate research symposium in physical and mathematical sciences, Washington University, St. Louis. 2-3 November 2002. (poster)

102. <u>M.C. Zwier*</u> and B.P Krueger. "Use of Molecular Dynamics Simulations in Analysis of Fluorescence-Detected Resonance Energy Transfer (FRET) Experiments." Pew mid-states undergraduate research symposium in physical and mathematical sciences, Washington University, St. Louis. 2-3 November 2002. (talk)

103. <u>C.J. Goltz*</u>, <u>J. Broyles</u>, <u>B.L. Mason*</u>, B.P. Krueger, and M.A. Burnatowska-Hledin. "Use of Steady-State and Time-Resolved Fluorescence To Characterize Vasopressin-Receptor Binding." Pew mid-states undergraduate research symposium in biological sciences, The University of Chicago. 26-27 October 2002. (poster)

104. <u>M.C. Zwier*</u>, and B.P Krueger. "Use of Molecular Dynamics Simulations in Analysis of Fluorescence-Detected Resonance Energy Transfer (FRET) Experiments." NSF-REU regional meeting, Kent State University. 31 July 2002. (poster)

WORKSHOPS

LibreTexts Workshops

1. Multi-day workshops at Hope College including instruction in the pedagogy of online resources, OERs in general, and LibreTexts in particular.   June 2019

2. Multi-day online workshops similar to above. International audience.

3. One-two day workshops targeted to a specific campus/region.

<div align="right">Oct 2020, Mar 2021</div>

WebMO for High School Teachers

1. One-week residential workshops at Hope College giving high school teachers instruction in quantum chemistry and WebMO and assisting them in developing a complete lesson for their classroom.   Summer 2009, 2010, 2011, 2012, 2013, 2015

TEACHING EXPERIENCE

Hope College Courses Taught

2. Chem 111 and 125 General Chemistry I (Dual numbering results from a complete redesign of our GenChem sequence in 2011).   Fall 2005, 2006

3. Chem 121 and 126, General Chemistry II.   Spring 2006, 2007, 2012, 2014, 2016

4. Chem 113 and 127, General Chemistry Laboratory I.
<div align="right">Fall 2002, 2003, 2004, 2009, 2010, 2011, 2013, 2014</div>

5. Chem 114 and 128, General Chemistry Laboratory II.
<div align="right">Spring 2002, 2003, 2011, 2012, 2014, 2015</div>

6. Chem 195, Day1: Watershed Laboratory (Research based Chem & Bio Lab).
<div align="right">Fall 2016, 2017, 2018, 2020</div>

7. IDS 100, First Year Seminar (accompanying Day1: Watershed Laboratory)
<div align="right">Fall 2016, 2017, 2018, 2020</div>

8. Bio 195, Day1: Watershed Laboratory (Research based Bio & Chem Lab).
<div align="right">Spring 2017, 2018, 2019, 2021</div>

9. Chem 195/295, Chemical Modeling Laboratory (Research-based Python Programming).
<div align="right">Spring 2017, 2019, 2021</div>

10. Chem 343, Physical Chemistry I (Statistical Thermodynamics & Kinetics).
<div align="right">Fall 2001, 2002, 2003, 2004, 2005, 2006, 2008, 2009, 2010, 2011, 2015, 2020</div>

11. Chem 344, Physical Chemistry II (Quantum Mechanics).
<div align="right">Spring 2009, 2014, 2015, 2016, 2017, 2018, 2019, 2021</div>

12. Chem 345, Physical Chemistry Laboratory I.
<div align="right">Fall 2001, 2008, 2013, 2014, 2015, 2016, 2017, 2018</div>

13. Chem 346, Physical Chemistry Laboratory II.
<div align="right">Spring 2002, 2004, 2009, 2010, 2011, 2016</div>

14. Chem 347, Chemical Modeling Laboratory.   Spring 2009, 2015

15. Chem 348, Advanced Spectroscopy.   Spring 2002, 2004, 2006, 2010

16. Bio 395/Chem 395, Methods in Modeling Complex Systems (cross-listed).

17. Chem 422, Structure, Dynamics, and Synthesis II (group theory, statistical mechanics, and other advanced topics in PChem).　　　　Spring 2002, 2003, 2004, 2006, 2009

18. Chem 490, Independent Research in Chemistry.
　　　　　　　　　　　　　　　　　　Spring and Fall 2001-present

19. Bio495/Chem495, Journal Club in Structural Biology (cross-listed).　　Spring 2004, 2006

20. Chem795/Educ795, Computational Chemistry and Inquiry (cross-listed).
　　　　　　　　　　Summer 2009, 2010, 2011, 2012, 2013, 2015

Hope College Curriculum Development

1. Co-developed Programming Foundations with Application Modules, which is a suite of Course-based Research Experience modules spanning multiple departments and divisions. See Chem 195/295, Chemical Modeling Laboratory above.　　2015–present

2. Refined and added Learning Goals/Skills Mapping to the suite of Day1: Watershed courses, with Dr. Aaron Best and Dr. Catherine Mader.　　　　2016–present

3. Chaired General Chemistry Laboratory curriculum redesign committee, which completely redesigned the GenChem lab sequence, Chem 127 and 128.　　2010–2011
　　And implemented new curriculum by coordinating Chem 127 and 128.　　2011–2012

4. Rewrote three lab manuals due to redesign of the Chem 127 and 128 courses and a new Chem 132 course.　　　　　　　　　　　　2010–2011

5. Chaired In-depth Chemistry Curriculum Committee, which examined possible in-depth courses to fit new ACS guidelines.　　　　　　　　Spring 2010

6. Member of Biochemistry subgroup of Chem Dept curriculum reform.　　Fall 2010

7. Developed week-long intensive workshop to teach high school teachers about molecular modeling and inquiry-based instruction, Chem795 and Educ 795.　2008–2009

8. Developed interdisciplinary Methods in Modeling Complex Systems course with Dr. Aaron Best.　　　　　　　　　　　　Spring 2007

9. Gradually redesigned Physical Chemistry I Lecture to include biological examples suitable for students in the Biochemistry and Molecular Biology major. (Extensive redesign contributed by Dr. William Polik in Fall 2007.)　　　　2001–present

10. Developed a new Raman spectroscopy experiment for the Advanced Spectroscopy course.　　　　　　　　　　　　　　　　Spring 2004

11. Developed a new experiment for Physical Chemistry I, utilizing fluorescence quenching to measure thermodynamics of binding (with Dr. Michael Pikaart).　　2004–2006

12. Developed new computational modeling/VSEPR experiment for the General Chemistry I laboratory course (with Dr. Sheldon Wettack).　　2005–2006

University of California at San Francisco Courses Taught

1. Chem 111, Physical Chemistry Laboratory I.   Fall 2000

2. Chem 112, Physical Chemistry Laboratory II.   Spring 2001

Other Teaching Experience

1. Graduate student member, Teaching Matters Committee, The University of Chicago.
                                                                1994–1996

2. General Chemistry Teaching Assistant, The University of Chicago.   1993–1994
   Co-initiated and implemented a *Chemistry in Art* field trip to Art Institute of Chicago.

3. Organic Chemistry Teaching Assistant, Truman State University.   1991

PROFESSIONAL SERVICE

Reviewer

1. National Science Foundation MRI Spectroscopy/Microscopy review panels.
                                              April 2012, May 2014, Mar 2018

2. Member of the National Science Foundation TeraGrid Allocations Committee,
   quarterly review panel for supercomputer centers.   2008–2011

3. External reviewer for tenure, promotion and/or internal grants, five times.   2008–2013

4. Ad hoc reviewer for funding agencies, including: National Science Foundation,
   American Chemical Society-Petroleum Research Fund, Research Corporation, Murdock
   Charitable Trust.

5. Journals including: Proceedings of the National Academy of Sciences, USA; Journal
   of the American Chemical Society; Journal of Physical Chemistry A & B; Biophysical
   Journal; Journal of Computational Chemistry; Journal of Chemical Physics; Chemical
   Physics Letters; Biochemistry; The Chemical Educator.

6. The Council on Undergraduate Research, Posters on the Hill.   Jan 2011

Meetings and Organizations

1. Midwest Undergraduate Computational Chemistry Consortium (MU3C).   2002–present
   - Co-founder 2002, co-leader 2002–present.
   - Cluster administrator 2009–present.
   - Organizer of annual summer research symposia three times:
     - 2003, held at Northwestern University hosted by Mark Ratner.
     - 2004, held at University of Wisconsin-Madison hosted by Jim Skinner.
     - 2005, held at University of Minnesota hosted by Chris Cramer.
   - Promotes student-driven computational chemistry research at primarily
     undergraduate institutions in the Midwest.

- Provides access to cluster hardware and computational chemistry software.
- Annual summer research symposia focus on undergraduate student talks and allow students to network with university faculty such as Mark Ratner, Todd Martinez, Nancy Makri, Jim Skinner, Chris Cramer, Laura Gagliardi, Mark Gordon, Benoit Rouix, Charlie Brooks, Greg Voth.
- Annual winter online symposia.

2. ACS National Meeting session co-chair and co-organizer, *Connecting Computation to Experiment using Combined QM and MM Methods*. Salt Lake City, UT.   23 March 2009

3. ACS National Meeting session chair, *Molecular Mechanics in Proteins*. Dallas, TX.
<div align="right">18 March 2014</div>

Professional Affiliations

1. American Association for the Advancement of Science.

2. American Chemical Society.

3. American Physical Society.

4. Biophysical Society.

5. American Society for Biochemistry and Molecular Biology

6. Midwest Undergraduate Computational Chemistry Consortium.

HOPE COLLEGE SERVICE

Campus Service

1.	Presidential Transition Committee	2018–2019
2.	Faculty Compensation Task Force	2018–2020
3.	Global Partnerships Task Group for Internationalization of the Curriculum	2017
4.	Animal Care and Use Committee	2015–2019
5.	Board of Trustees, Faculty Representative	2014–2018
6.	Committee on Campus Climate	2014–2015, 2017-18
7.	Academic Affairs Board	2010–2012

- One of three primary campus governance boards.
- Chair 2011–12. Many major items were acted upon including:
  - Complete redesign of the Global Learning component of the General Education curriculum.
  - Restructuring of Social Science component of the General Education Program.
  - Extensive discussion which laid the foundation for action in 2012-2013 to implement a campus-wide approach to writing.
  - Held campus-wide discussion regarding grade inflation and possible mechanisms for improved feedback to students.
  - Also discussed or reported on items such as possible revision of the Academic Schedule, First-year Learning Communities, appropriate use of Dashboard data, the FYS program, and the Internship program.

- Secretary 2010-11.

8. Member of divisional Diversity Task Force. Spring 2011, 2011-12

9. Member, Financial Response Team. Chosen by Provost to determine Fall 2010
ways to reduce cost and improve quality of the academic program.

10. Director of the Computational Science and Modeling Laboratory. 2005–present
   - Building planning committee 2002. (except 07–08)
   - Cluster acquisition committee 2004–2005.
   - Provides high-performance computing capability for research and teaching to all
     faculty in the National and Applied Sciences Division. From mid-2009 through
     2012 the Computational Science and Modeling Laboratory enabled:
       - Ten courses supporting ~460 students per year.
       - Seventeen peer-reviewed publications.
       - $ 3.8 million in external funding.

11. Committee on Admissions and Financial Aid. 2003–2010 (except
   - Chair 2008-2010. Implemented programs to spring 05 and 07–08)
     improve recruitment of diverse students.
   - Secretary 2003-04, 2006-07.

12. Alternate, Human Subjects Review Board 2011–2018
(except 12-13)

13. Member, Human Subjects Review Board. 2009–2011
   - Participated in extensive redesign of procedures and documentation in 2011.

14. Chair, integrated science curriculum committee. Spring 2002

15. Member, Howard Hughes Medical Institute grant proposal committee. Fall 2002

Departmental Service (selected items)

1. Admissions Liaison Committee 2018–2019

2. Executive Committee Member 2017–2019

3. Schaap Funding Committee 2017–2018

4. Course Scheduling Coordinator 2014–2018

5. Chaired General Chemistry Textbook Selection Committee. 2013–14

6. Chaired First-year Laboratory Coordinator search. 2013

7. Coordinated General Chemistry Laboratory program during the 2011–12
first year of implementation following comprehensive redesign.

8. Coordinated General Chemistry Laboratory program. 2010–11, 2014–15

9. Led departmental seminar program. 2003–04, 2009–10, Fall 2010

10. Department liaison for Hypercube Scholar award. 2001–2017

11. Administered several departmental instruments. 2001–present

12. Academic advisor for 10-20 students each year. 2001–present

Outreach

1. Co-advisor 3rd Coast Cubing Club 2017–2019
2. Co-organized visit of high school students to Day1:Watershed course. 2017–present
   - Hamilton High School.
3. Molecular Modeling Workshop for high school teachers. 2009–2013
   - Developer, Administrator, and Lead Instructor.
   - One-week workshop brings 8–12 high school teachers to campus each summer.
   - Teachers develop lessons using molecular modeling and inquiry-based methods.
   - Since inception, 52 teachers have taught lessons to more than 5,000 students who have executed more than 50,000 quantum calculations. Many of these teachers continue to use these lessons each year.
   - Assessment results demonstrate an increased desire to attend college (39%) and to pursue careers in science (29%) and computing (25%).
4. Guest speaker in elementary classrooms.
5. Speaker for Hope Science Day program.

COMMUNITY SERVICE

Grace Episcopal Church
- Stewardship 2013–2018
- Budget preparation team 2013–2018
- Senior Warden 2015
- Vestry member 2013–2015