Brent P. Krueger

Towsley Research Scholar
Assistant Professor
Hope College
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ACADEMIC POSITIONS

2001- Assistant Professor of Chemistry, Hope College, Holland, MI 49423
2004-7 Towsley Research Scholar, Hope College

EDUCATION

1999 Ph.D. in Physical Chemistry, 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, University of Chicago.

1993 B.S. in Chemistry and Physics, *summa cum laude*, Truman State University, Kirksville, MO.

SELECTED RESEARCH SUPPORT

(Total support since 2001: $491,809 and 440,000 hours)

2005-8 National Science Foundation. *Acquisition of a Computer Cluster for Research, Research Training, and Teaching*. Co-PI with William Polik (Hope), Daniela Kohen (Carleton), Kieth Kuwata (Macalester), and Jonathan Smith (Gustavus-Adolphus). $ 379,609.

2005-7 American Chemical Society Petroleum Research Fund. *Simulating Linear and Nonlinear Optical Spectra in Condensed Phase Systems with a Mixed Molecular Dynamics and Quantum Mechanical Method.* $ 35,000.

2005-6 TeraGrid. *Using replica exchange molecular dynamics to evaluate dynamic contributions to fluorescence-detected resonance energy transfer (FRET) experiments in hen egg-white lysozyme*. 30,000 hours.

2004-6 National Center for Supercomputing Applications. *Evaluation of a mixed molecular dynamics and quantum mechanical method for simulating linear and nonlinear optical spectra in condensed phase systems.* 200,000 hours.

2004-7 Hope College Towsley Research Scholar Award. *Understanding Disease and Treatment by Understanding Protein Function: Developing New Biophysical Tools in Structural Biology.* One semester sabbatical and $ 16,000.

2002-4 Research Corporation. *Protein-protein interactions studied through 1-d and 2-d fluorescence lifetime spectroscopy and molecular dynamics calculations.* $ 45,200.

SELECTED FELLOWSHIPS AND SCHOLARSHIPS

2004-07 Towsley Research Scholar, Hope College.

2000-01 NIH Postdoctoral Fellow, University of California at San Francisco.

1999 Dutch Visiting Research Fellow, Free University, Amsterdam, The Netherlands.

1996-98 McCormick Fellow, University of Chicago.

1993-96 Department of Defense National Defense Science and Engineering Graduate Fellow.

1988-92 President's Honorary Full Scholar, Truman State University.

RESEARCH TRAINING

1999-2001 **Postdoctoral Research with Professor Peter A. Kollman.**
Department of Pharmaceutical Chemistry, University of California at San Francisco.
Molecular Dynamics Studies of Structure-Function Relationships in Proteins. Analyzed stability of a highly-charged, highly-conserved peptide from an SH3 domain, revealing possible sequence-function relationships for protein folding. Examined flexibility of mercuric ion reductase carboxy-terminal loop in relation to proposed functional mechanisms.

1999 **Dutch Visiting Research Fellowship with Professor Rienk van Grondelle.**
Department of Physics and Astronomy, Vrije Universiteit, Amsterdam, The Netherlands.
Spectroscopic Studies of Peridinin-Chlorophyll-Protein and CP29. Performed polarized transient absorption experiments to investigate light-harvesting function in peridinin-chlorophyll-protein and assisted development of a three-pulse photon echo spectrometer for studying pigment-protein interactions in CP29.

1993-99 **Graduate Research with Professor Graham R. Fleming.**
Department of Chemistry and the James Franck Institute, University of Chicago (1993-97).
Department of Chemistry, University of California, Berkeley and
Physical Biosciences Division, Lawrence Berkeley National Laboratory (1997-99).
The Role of Carotenoids in Bacterial Light-Harvesting. Utilized a variety of time-resolved spectroscopies to measure energy transfer timescales in photosynthetic light-harvesting antenna. Developed *ab initio* methods to fully describe resonance Coulombic coupling in these systems.

1995 **Department of Defense Summer Fellowship with Dr. Mike Duncan and Dr. Mark Seaver.**
Optical Sciences Division, Naval Research Laboratory, Washington D.C.
Construction of Near-Field Scanning Optical Microscope. Finished construction of near-field scanning optical microscope for use in detection of fluorescent-labeled DNA.

1992 **Undergraduate Summer Research Fellowship with Professor John Jean.**
Department of Chemistry, Washington University.
Characterization of CdS nanoclusters. Utilized a variety of steady-state spectroscopies to characterize the electronic properties of CdS nanocrystals.

TEACHING EXPERIENCE

2001- **Assistant Professor**, Department of Chemistry, Hope College.
Courses Taught: Physical Chemistry I (Statistical Thermodynamics & Kinetics); Physical Chemistry Laboratory I & II; General Chemistry I; General Chemistry Laboratory I & II; Structure, Dynamics, and Synthesis II (advanced topics in PChem); Advanced Spectroscopy; Journal Club; Independent Research in Chemistry.
Also headed development of an interdisciplinary minor, Computational Science and Modeling, along with a high performance computing facility. Currently serving as supervisor of the Computational Science and Modeling Facilitator who administers the laboratory.
Developed new laboratories for Advanced Spectroscopy, Physical Chemistry Laboratory I, and General Chemistry I.
Complete teaching evaluations available on request (nationally-normed SIR-II). In summary, I have received 18 evaluations with enough students to be statistically significant. Of the 112 total categories that were scored, I was rated statistically above the mean in 4, above the mean in 93 and below the mean in 15. In the *Overall Evaluation* category where students "Rate the quality of instruction in this course as it contributed to your learning" I was rated statistically above the mean once and above the mean the remaining 17 times.

2000-01 **Faculty Laboratory Instructor**, Physical Chemistry Chem 111 & 112,
Pharmaceutical Chemistry Department, University of California, San Francisco.
Lectured and demonstrated material, primarily thermodynamics and kinetics, for laboratory section. Included use of computerized lecture room for molecular modeling.

1994-96 **Graduate Student Member**, Teaching Matters Committee, University of Chicago.
Represented graduate students for course planning and student awards.

1993-94 **Teaching Assistant**, General Chemistry, Department of Chemistry, University of Chicago.
Led recitation section and review sessions and supervised laboratory. With one other T.A. initiated and implemented a *Chemistry in Art* field trip to the Art Institute of Chicago.

1991 **Teaching Assistant**, Organic Chemistry, Department of Chemistry, Truman State University.
Assisted professor in supervising laboratory and recitation.

2000 **Coach**, sixth through eighth grade boys basketball, Saklan Valley School, Moraga, CA.
Performed all coaching duties for middle school basketball team.

1997-99 **Guest Lecturer**, eighth grade science class, Saklan Valley School.
Gave presentations on photosynthesis, light and lasers including hands-on demonstrations.

1995-97 **Volunteer Science Partner**, University of Chicago and Chicago Public Schools.
Assisted elementary school teachers by performing science demonstrations. Also judged science fair projects for disadvantaged junior high school.

1996-97 **Private Tutor**, Chicago, IL.
Tutored high school students in chemistry and calculus.

1990-93 **Volunteer Tutor**, Science Division, Truman State University.
Tutored college students in chemistry, physics, and calculus.

AFFILIATIONS

American Physical Society
American Chemical Society
Biophysical Society
Council on Undergraduate Research
American Association for the Advancement of Science

PUBLICATIONS (UNDERGRADUATE AUTHORS INDICATED BY *)

1. 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).

2. 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).

3. 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).

4. 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).

5. 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).

6. Carotenoid Mediated B800-B850 Coupling in LH2. B.P. Krueger, G.D. Scholes, I.R. Gould, and G.R. Fleming. *PhysChemComm*. **8** (1999). http://www.rsc.org/ej/qu/1999/C9903172/index.htm.

7. 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).

8. 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).

9. 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).

10. 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, D. Rutkauskas*, R.G. Hiller, and R. van Grondelle. *Biophys. J.* **80**, 2843-2855 (2001).

11. 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).

12. 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).

13. Photochemistry. G. R. Fleming, J. W. Longworth, and B.P. Krueger. In: *Encyclopedia Brittanica Online*.

14. 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).

15. 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).

16. 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.* in press.

17. A Thermodynamic Exploration of Eosin-Lysozyme Binding: A Physical Chemistry and Biochemistry Laboratory Experiment. A.J. Huisman*, L.R. Hartsell*, M.J. Pikaart, and B.P. Krueger. manuscript in preparation for *J. Chem. Ed.*

18. Evalulation of a Hybrid Molecular Dynamics and Quantum Mechanics Method for Simulating Solvation Dynamics. Matthew C. Zwier*, Justin M. Shorb*, and Brent P. Krueger. manuscript in preparation.

19. Computational Analysis of the Assumptions Underlying the Use of FRET as a Spectroscopic Ruler. D. Van Beek*, Matthew C. Zwier*, Justin M. Shorb*, and Brent P. Krueger. manuscript in preparation.

RESEARCH PRESENTATIONS

1. Applications of Ultrafast Spectroscopy in Biology and Solution. Student Poster Session, University of Chicago, Chicago, IL. February 1996. (poster)

2. 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)

3. The Role of Carotenoids in Bacterial Light-Harvesting. Tenth Annual Western Photosynthesis Conference. Asilomar Conference Center. 6 January 1999. (talk)

4. Two-photon Fluorescence Excitation Spectra of the S_1 State of Spheroidene and the Role of the Carotenoid in Promoting B800 to B850 Energy Transfer in LH2. Informal Seminar, Lund University, Lund, Sweden. Hosts: J. Herek and V. Sundström, June 1999. (talk)

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

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

7. 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)

8. 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)

9. 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 presented by undergraduate student Matthew C. Zwier)

10. 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 presented by undergraduates Christopher J. Goltz and Beauregard L. Mason)

11. 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 presented by undergraduate student Darren VanBeek)

12. 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 presented by undergraduate student Timothy R. Stowe)

13. Modeling the Behavior of Siloxane Polymers as Emulsifiers using Molecular Dynamics Simulations. 37th Silicone Symposium, University of Pennsylvania, 19-21 May 2004. (poster presented by undergraduate student Justin M. Shorb)

14. 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 presented by undergraduate student Darren VanBeek)

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

INVITED LECTURES

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

2. Echos of Light: Nonlinear Ultrafast Spectroscopy. Chemistry Dept., Truman State University. 29 October 1998.

3. Understanding photosynthesis through non-linear spectroscopy and computations. Structural Biology Seminar, University of Minnesota. 24 September 2001.

4. Examining Phospholamban Binding Through Time-resolved Fluorescence and Computations. Informal Seminar, University of Minnesota, Host: D. Thomas, 24 September 2001.

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

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

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

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

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

10. Can physics and biology get along? Using spectroscopy and computation to study regulation, Science Division Colloquium, Calvin College, 4 December 2003.

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

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

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

14. Can physics and biology get along? Developing new tools for structural biology through spectroscopy and computation. Chemistry Seminar, Grand Valley State University, 8 April 2005.

15. 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.