

# Justin M. Shorb

CURRICULUM INNOVATION · OPEN EDUCATIONAL RESOURCES CURATOR · SCIENCE EDUCATION RESEARCHER

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*“The test of a good teacher is not how many questions he can ask his pupils that they will answer readily, but how many questions he inspires them to ask him which he finds it hard to answer.” - Alice Wellington Rollins*

## Education

### 2011 Ph.D. Chemistry Education and Theoretical Physical Chemistry

University of Wisconsin - Madison

ADVISORS: JOHN W. MOORE AND JAMES SKINNER

Madison, WI

Thesis: Development and Implementation of an Empirical Frequency Map for use in MD Simulation of Isotope-Edited Proteins AND Development, Implementation, and Evaluation of an Online Student Portal as a Textbook Replacement in an Advanced General Chemistry Course

### 2004 B.S. Chemistry; B.A. Mathematics

Hope College

AMERICAN CHEMICAL SOCIETY CERTIFIED; *Cum Laude*

Holland, MI

## Professional Experience

### Director of Curriculum Innovation and Development

Washington, DC

LIBRETEXTS, INC.

2024 – Present

Joshua Halpern, Ph.D., Chief Operating Officer

- Designing training materials, workshops, and mentoring of authors/instructors throughout the LibreTexts Consortium.
- Collaborate on assessment of learning and user experience research.
- Product Manager and Owner for new technologies on the LibreTexts Platform.

### Product Manager and OER Library Curator

Austin, TX

CATALYST EDUCATION, LLC (LABFLOW)

2020 – 2024

- Managed at team of Ph.D. Chemists in developing and refining online laboratory manual materials for an OER Library as well as Custom solutions for over 50,000 students in an academic year.
- Designed the template for both print and online laboratory manuals using  $\LaTeX$
- Organized distribution of OER Lab materials to partner organizations: OpenStax and LibreTexts.
- Collaborated on ongoing company research into efficacy of teaching materials as well as curriculum design.

### Instructor of Chemistry and General Chemistry Laboratory Coordinator

Durham, NC

DUKE UNIVERSITY

2022 – 2023

Charlie Cox, Ph.D., Director of Undergraduate Studies

- Revamping existing curriculum to improve efficiency in grading, administration, and training of both students and TAs.
- Instructor of Record for over 1200 students in 78 sections of 5 courses in two semesters.

### Assistant Professor of Chemistry and First-Year Laboratory Coordinator

Holland, MI

HOPE COLLEGE

2014 – 2020

Chairs: William Polik; Kenneth Brown; Elizabeth Sanford.

- Successful externally-funded research program including funding for a minimum of 4 research students per summer.
- Research areas include assessment of laboratory programs, online educational resources, eye tracking, and student interfaces.

### Assistant Professor of Chemistry

St. Thomas, USVI

UNIVERSITY OF THE VIRGIN ISLANDS

2011 – 2014

Chair: Stanley Latesky, Ph.D.

- Research areas included integration of water-testing chemistry into GenChem Lab, and student interfaces using eye-tracking.
- UVI is a Land Grant Institution and Historically Black College and University (HBCU) designated institution.

## **Instructor of Chemistry and Mathematics**

SINTE GLESKA UNIVERSITY, ROSEBUD SIOUX RESERVATION

*Chair: Godfrey Loudner, Ph.D.*

- Instructor-level teaching-only appointment including autonomous course design and instruction.
- SGU is a Tribal College and Universities (TCU) designated institution.

*Mission, SD*

*2004 – 2005*

## **Research Activities**

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### **Collaborator, Undergraduate Student Research**

DUKE UNIVERSITY

*Durham, NC*

*2022 - 2024*

- Consulted with the Cox Research Group on undergraduate research projects to assess the efficacy of online course preparation materials in the general chemistry laboratory.
- Co-authored a paper on learning in the organic chemistry lecture with undergraduate research students.

### **Curator of the Open Educational Resources (OER) Library of Chemistry Labs**

CATALYST EDUCATION, LLC (LABFLOW)

*Austin, TX*

*2020 - Present*

- Developed a set of Broader Topics of Learning Objectives and aligned the existing materials with research in General and Organic Chemistry Laboratory curricula.
- Trained five people in the writing of Learning Objectives, alt-text for accessibility, and  $\text{\LaTeX}$  editing.

### **LibreText Open Educational Resources HyperLibrary Project**

HOPE COLLEGE AND UNIVERSITY OF CALIFORNIA-DAVIS

*Holland, MI*

*2005 - Present*

- **Maintained active federal funding from October 2015 until present, with sustained federal funding until September 2020**
- Ported the ChemPRIME wiki textbook from the ChemEd DL into the LibreText to expand the former ChemWiki textbook offerings (now the Chemistry LibreText).
- Performed an analysis of existing hardcopy textbooks in comparison with ChemPRIME textbook based on content coverage using the ACS Examinations Institute published concept inventories as well as multimedia using the triplet relationship. Manuscript Drafted.
- Performed an analysis of the natural usage internal hyperlinks of website visitors and assessed their correlation of use with the author context and content relationships. Manuscript in Revision.
- Co-led training workshop at the Biennial Conference in Chemistry Education in designing online materials. • Recruiting non-chemists from across the country to attend train-the-trainer workshops to facilitate dissemination of the LibreText platform beyond the chemical sciences.
- Continued work with Catalyst Education, LLC, as the Curator of the OER Library.

### **Incorporation of Electronic Laboratory Notebooks into Introductory Health Sciences Course to Increase Authenticity**

HOPE COLLEGE

*Holland, MI*

*2016 – 2020*

- Designed an implementation of LabArchives ELNs in a first-year health sciences chemistry laboratories.
- Mentored a post-baccalaureate student in designing educational research protocols, literature, and experimental design.
- Continued mentoring through Amber (Prins) Dood's successful completion of a Ph.D. in Chemistry Education Research (University of South Florida; Advisor Jeff Raker), and then onward into her Postdoctoral work (University of Michigan; Mentor Ginger Schultz).

### **Maintainer and Curator of the Chemistry Education Digital Library**

HOPE COLLEGE; CATALYST EDUCATION, LLC

*Holland, MI*

*2015 – 2020*

- The ChemEd DL houses interactive learning materials for the chemical fields such as tutorials on stereochemistry, molecule viewers, and an interactive Periodic Table: PTL! The site has over 80,000 visitors per year.
- Mentored three undergraduate research students over two years.

### **Validation of a Novel Eye-Tracking Analysis Method**

*St. Thomas, USVI; Holland, MI*

UNIVERSITY OF THE VIRGIN ISLANDS; HOPE COLLEGE

2095 – 2020

- Reproduced expert vs. novice experiment in multimedia chemistry education while incorporating eye-tracking to validate a principle-component analysis method of analyzing transition frequencies, as well as Artificial Intelligence Algorithms. Manuscripts Drafted.
- Mentored seven undergraduate research students over five years.

### **Development of the Science Laboratory Assessment Framework**

*Holland, MI*

HOPE COLLEGE

2095 – 2020

- Designed a framework for evaluating science laboratories which has been implemented at Hope College in Biology, Chemistry, and a new Watershed Lab, as well as in General Chemistry and Organic at St. Mary's College of Maryland. Manuscript Submitted.
- Developed new laboratories based on the evaluation outcomes.
- Mentored three undergraduate research students over two years.

### **Assistant Professor of Chemistry**

*St. Thomas, USVI*

UNIVERSITY OF THE VIRGIN ISLANDS

2011 – 2014

- Co-author of the successful EPSCoR Capacity Building grant and Systems Administrator of the installation of the Super-computer Cluster on UVI's campus.
- Advisory Board for Divergent-thinking intervention research program for incoming students.
- Part of design team for incorporating UTeach (from University of Texas at Austin) STEM curriculum into UVI's Educational Program.
- Co-designed and evaluated a peer-leadership program for introductory chemistry on both islands.
- Research areas included integration of water-testing chemistry into General Chemistry Laboratory, online-textbook development and student interfaces using eye-tracking, and computational exercises for teaching.
- Member of the UVI Website Redesign committee.
- Mentored five undergraduate research students over two years.

### **Graduate Research Assistant in Chemistry Education**

*Madison, WI*

UNIVERSITY OF WISCONSIN – MADISON

2095 – 2011

*Mentor: John W. Moore, W.T. Lippincott Professor of Chemistry*

- Developed an online textbook substitute by integrating interactive videos, animations, and molecule viewers from the ChemEd DL into a digitized version of Chemistry by Moore, Stanitski, and Davies.
- Evaluated the use of an online textbook using pre-/post-testing, quantitative, and qualitative measures. • Began work with eye-tracking to determine interaction of students with an emphasis on the use of the triplet relationship in chemistry.

### **Graduate Research Assistant in Theoretical Physical Chemistry**

*Madison, WI*

UNIVERSITY OF WISCONSIN – MADISON

*Mentor: James Skinner, Joseph O. Hirschfelder Professor of Chemistry (now: Crown*

2095 – 2011

*Family Professor of Molecular Engineering, Director of the Water Research Initiative and Deputy Dean for Faculty Affairs at University of Chicago*

- Developed an empirical mapping between electrostatic force and amide-I IR frequency for N-methylacetamide.
- Developed a parallel implementation of this empirical mapping code for generating frequency trajectories during MD simulations of peptides in GROMACS, with published work simulating the 2D-IR spectra of trans-membrane protein: CD3ζ.
- Wrote a program for scanning geometric rearrangements of molecules to develop force-field parameters for MD simulations.

### **Student Intern in Computational Chemistry Research**

*San Diego, CA*

SAN DIEGO SUPERCOMPUTER CENTER

*Mentor: Mentor: Prof. Ross Walker, HTC Consultant and Staff Scientist, Associate*

2095 – 2011

*Research Professor at SDSC.*

- Six-week internship learning how to utilize SDSC supercomputer clusters for computational research. Expanded Skinner Group analysis code to utilize parallel algorithms.



## Grants & Awards

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### EXTERNALLY FUNDED

- 2018 **Department of Education Fund for the Improvement of Postsecondary Education — Open Textbooks Pilot Program**  
Collaborative Research: Developing and Assessing Effective Cyberlearning within the STEMWiki Hyperlibrary (NSF DUE: 1524990)  
First-of-its-kind grant awarded \$4.9 million to a large consortium of colleges and universities led by Lead PI Delmar Larson at UC-Davis. \$161,000 over three years awarded to Hope College as the hub for a train-the-trainer workshop in spreading LibreText to other non-chemistry disciplines and evaluating its dissemination.
- 2017 **Society for Analytical Chemists of Pittsburgh (SACP) Education Award**  
Support for the ongoing Chemistry Education Digital Library hosted at Hope College) ([www.chemeddl.org](http://www.chemeddl.org))  
Small award for the continued building and maintenance of the Chem Ed DL.
- 2017 **Hellma, USA, Collaboration**  
Courseware for the REVA Educational Raman Platform ([www.learnraman.com](http://www.learnraman.com)) (Prototype Instrument is in my possession)  
Funding for PI and an undergraduate researcher to collect data on what laboratories would be marketable to include with a new Raman spectroscopy instrument for teaching labs, test and design the labs, and write up laboratory instructions, prep notes, and accompanying template spreadsheets. Published eight Raman Laboratories for General, Organic, Analytical, Geochem, Inorganic, and Physical Chemistry labs (view at link above).
- 2016 **Michigan Space Grant Consortium (MSGC) Research Seed Grant**  
Establishing Validity of a Novel Eye-Tracking Data Analysis Method to Chemistry Education Research and its Application to the Evaluation of Online Chemistry Teaching Materials (\$5000 awarded, \$5000 internal funding match)  
[A portion of this grant was used to purchase an Eye-Tracker, which is still in my possession.](#)
- 2015 **National Science Foundation Improving Undergraduate STEM Education (NSF IUSE)**  
Collaborative Research: Developing and Assessing Effective Cyberlearning within the STEMWiki Hyperlibrary (NSF DUE: 1524990)  
Hope College's role was to port the ChemPRIME textbook from ChemEd DL to the LibreText in its entirety and to evaluate the traffic and multimedia usage of the textbooks. \$39,500 awarded over two years.
- 2015 **National Science Foundation Experimental Program to Stimulate Competitive Research (NSF EPSCoR)**  
VI-EPSCoR: RII: Building Research Strength in the US Virgin Islands (NSF EPS: 0814417)  
Left UVI before grant was awarded. Listed as Senior Personnel and wrote a large portion of the budget (\$5 million) of a \$12.5 million grant that was awarded. The portions I was involved in consisted of teacher training, workforce development, laboratory development, and the creation of a new Institute for STEM Education Research and Practice.

### INTERNALLY FUNDED

- 2015 **Hope College HHMI Faculty Research Award**  
Establishing Validity of a Novel Eye-Tracking Data Analysis Technique to Chemistry Education Research and Application to Online Chemistry Laboratory Prelab Material (\$8,355 plus funding for one additional undergraduate research student)  
[Competitive Faculty Research Funding from an HHMI Stimulating Undergraduate Research Program \(2012\)](#)

## Teaching Experience

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### Instructor of Chemistry and General Chemistry Laboratory Coordinator

Durham, NC

DUKE UNIVERSITY

2022 – 2023

- Coordinate all general chemistry laboratory sections including creating a Grad Student TA Training program weekly training, and coordinating online materials and grading consistency for both online and in-person labs.
- Courses taught: Introduction to Biological Chemistry for the Allied Health Fields Lab; General Chemistry Lab and Lecture; Physical Chemistry Lecture.
- General Chemistry Laboratory, Applications in Modern Chemistry Lab, Honors General Chemistry Lab

### Assistant Professor of Chemistry and First-Year Laboratory Coordinator

Holland, MI

HOPE COLLEGE

2014 – 2021

- Coordinate all first-year laboratory sections including creating a Lab TA Training program, Instructor weekly training, and coordinating laboratory prep for all 300+ students.
- Courses taught: Introduction to Biological Chemistry for the Allied Health Fields Lab; General Chemistry Lab and Lecture; Physical Chemistry Lecture.
- Guest Instructor in Inorganic Chemistry Lab, and Advanced Spectroscopy Lab.

### Assistant Professor of Chemistry

St. Thomas, USVI

UNIVERSITY OF THE VIRGIN ISLANDS

2011 – 2014

- Courses Taught: General, Organic, and Biochemistry for Nursing Chemistry Lecture and Lab; General Chemistry Lecture and Lab; Physical Chemistry Lecture and Lab; Junior Seminar; Senior Seminar.

### Teaching Assistant GenChem II & Honors Advanced GenChem

Madison, WI

UNIVERSITY OF WISCONSIN – MADISON

2008

*John Berry (104), John W. Moore (109H), Arun Yethiraj (115/116), and Claude Woods (115/116)*

- Supervised one lab session and one discussion per week for two sections in 104, and in one section for 109H.
- Directed students in one discussion and two laboratories per week. Class was the top 30 students of the 3000 student cohort of first-year chemistry students and was physical-chemistry-based curriculum. Reorganized lab schedule and rewrote MathCad handouts. Created and maintained a website for 116.
- Substitute lecturer for Yethiraj.

### Developer of the TA Grade Report E-mailer (TAGRE)

Holland, MI

UNIVERSITY OF WISCONSIN – MADISON

2014 - 2021

*Chad Wilkinson, General Chemistry Laboratory Director*

- Designed a pHp-based website which generated personalized e-mails with grades and feedback for each student for each lab, while updating a central repository of grades. Utilized by over 100 TAs per semester, and is still used at UW-Madison over a decade later!

### Instructor of Chemistry and Mathematics

Mission, SD

SINTE GLESKA UNIVERSITY

2004 - 2005

- Near-autonomous curriculum development and instruction of General Chemistry I & II (with labs), College Pre-Algebra, and Discrete Mathematics for Computer Science: including textbook selection, lab/demo prep, lab manual creation.
- Full year of teaching with only B.S.

## Professional Activities and Honors

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05/16 – present: Member of LibreTexts Development Team

02/16: Hope College Faculty Technology Innovation Award Runner-Up

05/15 – 07/21: Member of Hope College Safety Committee

05/15 – 05/18: Member of Hope College Assessment Committee

08/14 – 07/18: Member of Hope College Chemistry Department Assessment Committee

05/12 – 07/14: Member of the UVI Faculty Assessment Learning Community

02/13: Invited participant in POGIL-PChem Lab Workshop at Virginia Tech.

08/12: Selected as Faculty Mentor for UVI ACS Chem Club

08/12: Internal Funding for Peer Instruction implementation at UVI (Center for Student Success)

05/10: Outstanding Chemistry Teaching Award  
04/04: American Institute of Chemists Award  
04/03: Hypercube Scholar Award (in Computational Chemistry)  
09/03 – 05/04: Vice President of Hope College Chemistry Club  
05/00 – 05/04: Kalamazoo Science Foundation Scholarship

## Presentations

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### INVITED ORAL PRESENTATIONS

- 10/2017 **Do online materials actually increase student engagement? Establishing the validity of eye-tracking for evaluating online teaching materials in chemistry.**  
Great Lakes Local ACS Seminar Series  
[Grand Valley State University](#)
- 04/2015 **Using Eye-Tracking to Gain Insight into Student Understanding of Multiple Representations in Chemistry.**  
Natural Sciences Seminar Series  
[St. Mary's College of Maryland](#)
- 10/2017 **Using Eye-Tracking to Gain Insight into Student Understanding of Multiple Representations in Chemistry.**  
Chemistry Department Seminar Series  
[Grand Valley State University](#)
- 11/2014 **Using eye-tracking to determine student reading patterns of multiple representations: Development of a novel time-sensitive principal component analysis (PCA/Eigenvector) approach.**  
Natural and Applied Sciences Seminar Series  
[Manchester University](#)

### ORAL PRESENTATIONS

- 08/2018 **Multiple representations and understanding: Expert and novice responses to different representations of chemical phenomena and the use of quantitative data to validate eye-tracking experiments.**  
BCCE2018 Chemistry Education Workshop  
[Notre Dame, IN](#)
- 08/2018 **Development of a Science Laboratory Assessment Framework and its use in chemistry and interdisciplinary curriculum improvement.**  
BCCE2018 Current Research on the Undergraduate Chemistry Laboratory Symposium  
[Notre Dame, IN](#)
- 08/2016 **Social cognitive whole student (SCWS) framework for the design and evaluation of undergraduate STEM programs.**  
BCCE2016 Addressing underrepresented groups in STEM Symposium  
[Greeley, CO](#)
- 08/2016 **Establishing validity of a novel eye-tracking data analysis method for analyzing gaze patterns of multiple representations.**  
BCCE2016 Chemical Education Research Symposium  
[Greeley, CO](#)
- 08/2016 **Establishing validity of a novel eye-tracking data analysis method for analyzing gaze patterns of multiple representations.**  
BCCE2014 Chemical Education Research Symposium  
[Greeley, CO](#)
- 08/2014 **Establishing validity of a novel eye-tracking data analysis method for analyzing gaze patterns of multiple representations.**  
BCCE2016 Chemical Education Research Symposium  
[Allendale, MI](#)
- 08/2014 **Use of water quality tests as a foundation for a more inquiry-based general chemistry laboratory.**  
BCCE2016 Chemical Education Research Symposium  
[Allendale, MI](#)

- 05/2013 **Using Online Homework to Create Opportunities for Student-Centered Instruction.**  
201st Two Year College Chemistry Consortium (2YC3) Conference  
[Webinar](#)
- 08/2010 **Online textbooks are more than an online book: The development of ChemPaths online student portal.**  
ACS 240th National Meeting  
[Boston, MA](#)
- 08/2010 **ChemPRIME wiki-text: The chemistry behind your favorite subject.**  
BCCE2010  
[Denton, TX](#)
- 08/2010 **ChemPaths: Evaluation of an Online Portal to ChemEd Digital Library Resources for Intrinsically Linked Learning.**  
BCCE2010  
[Denton, TX](#)
- 10/2009 **Incorporating Multi-Sensory Education in an Advanced General Chemistry Course.**  
1st Annual Conference on Multi-Sensory Science Education  
[Madison, WI](#)
- 08/2008 **ChemPaths: Learning to Meander – An Online Portal to ChemEd DL Resources for Intrinsically Linked Learning.**  
ACS National Meeting Social Networking Symposium  
[Washington, DC](#)

## WORKSHOPS

- 08/2022 **Aligning Laboratory Experiments with Learning Objectives for Focused Formative Assessment.**  
BCCE2022  
[Purdue University](#)
- 07/2019 **Design and use of LibreTexts online hyperlibrary for use in the classroom by invitation at Saint Mary's College by invitation. 11 attendees.**  
LibreTexts Workshop on the Design, Use, and Building of online textbooks  
[Notre Dame, IN](#)
- 06/2019 **Design and use of LibreTexts online hyperlibrary for use in the classroom for Hope College and midwest colleges and community colleges. Two-day workshop for designing and building. 6 attendees.**  
Design and use of LibreTexts online hyperlibrary for use in the classroom.  
[Holland, MI](#)
- 05/2015 **Week-long workshop on pedagogical design of curricular materials and evaluation. Attended by Hope, GVSU, and University of the Virgin Islands faculty and Science Education Research students.**  
2015 SciEd Research Summit  
[Holland, MI](#)
- 08/2010 **Editing Wikipedia and the ChemPRIME General Chemistry Wiki (workshop co-leader).**  
BCCE2010  
[Denton, TX](#)
- 08/2010 **Using Social Networking in Chemical Education (workshop co-leader).**  
BCCE2010  
[Denton, TX](#)

## Publications

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\* - Denotes Undergraduate Research Student Author.

Liang-Lin, J.G.,\* T.R. Locascio,\* A. Witherspoon,\* S. Gao,\* J. Laster,\* M. Tripp,\* J.M. Shorb, C.T. Cox Jr. (2024). "How Much? How Fast? A Study of Kinetics and Thermodynamics Through the Lens of Reaction Coordinate Diagrams in Organic Chemistry." Journal of Chemical Education. 101, 6, 2308-2320

Lake, W.,\* E. Ropski,\* and J.M. Shorb. "Social Cognitive Intervention Framework with Whole-Student Outcomes: An Evaluation Framework for Designing, Evaluating, and Improving First-Year STEM Undergraduate Programs." Pending.



Lake, W.,\* J.R. Cerone,\* and J.M. Shorb. “Investigating the Validity of the Hypertext Theory of Learning via Website Analytics of Intratext Links in an Online Chemistry Library.” Pending.

Monson, K.,\* Y.C. Yoon,\* M. Charles,\* and J.M. Shorb. “Development of a Novel Transition Frequency Principle Component Approach for Eye-Tracking Data Analysis.” Pending.

Dood, A.,\* L. Johnson, and J.M. Shorb (2018). “Electronic Laboratory Notebooks Allow for Modifications in a GOB Chemistry Laboratory to increase Authenticity of the Student Experience.” In: Journal of Chemical Education.

Shorb, Justin M. (2011). Thesis: Development and implementation of an empirical frequency map for use in MD simulations of isotope-edited proteins, and, Development, implementation, and evaluation of an online student portal as a textbook replacement in an advanced general chemistry course. ISBN: 978-1-267-05340-4.

Shorb, J.M. and J.W. Moore (2010). “The ChemPaths Student Portal: Making an Online Textbook More than a Book On-line.” In: Enhancing Learning with Online Resources, Social Networking, and Digital Libraries. Vol. 1060. ACS Symposium Series 1060. American Chemical Society, pp. 283–308. ISBN: 978-0-8412-2600-5. DOI: 10.1021/bk-2010-1060.ch015. URL: <http://dx.doi.org/10.1021/bk-2010-1060.ch015>.

Lin, Y.-S., J. M. Shorb, P. Mukherjee, M. T. Zanni, and J. L. Skinner (2009). “Empirical Amide I Vibrational Frequency Map: Application to 2D-IR Line Shapes for Isotope-Edited Membrane Peptide Bundles.” In: The Journal of Physical Chemistry B 113.3, pp. 592–602. DOI: 10.1021/jp807528q. URL: <http://dx.doi.org/10.1021/jp807528q>.

Lin, Y-S, S G Ramesh, J M Shorb, E L Sibert, and J L Skinner (2008). “Vibrational energy relaxation of the bend fundamental of dilute water in liquid chloroform and d-chloroform.” In: The Journal of Physical Chemistry. B 112.2, pp. 390–398. ISSN: 1520-6106. DOI: 10.1021/jp075682s. URL: <http://www.ncbi.nlm.nih.gov/pubmed/18044869>.

VanBeek, D.B., M.C. Zwier, J.M. Shorb, and B.P. Krueger (2007). “Fretting about FRET: Correlation Between kappa and R.” In: Biophys. J. 92, pp. 4168–4178.

Zwier, M.C., J.M. Shorb, and B.P. Krueger (2007). “Hybrid Molecular Dynamics-Quantum Mechanics Simulations of Solute Spectral Properties in the Condensed Phase: Evaluation of Simulation Parameters.” In: J. Comput. Chem. 28, pp. 1572–1581.

## References Available upon Request

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Charlie Cox, Ph.D.

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919-660-1539 | [charlie.cox@duke.edu](mailto:charlie.cox@duke.edu)

Brent P. Krueger, Ph.D.

**Hope College**

Professor of Chemistry  
Developer/Instructor of the Watershed Day1 Research Community  
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Stanley Latesky, Ph.D.

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John W. Moore, Ph.D.

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