

Thomas E. Morrell

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(626)-395-3827 • tmorrell@caltech.eduorcid.org/0000-0001-9266-5146**Experience**

- Research Data Specialist**, Caltech Library, Pasadena, CA Jul. 2016-present
- Member of Digital Library Development group
 - Launched campus-wide research data repository, data.caltech.edu
 - Programs applications to manage library and campus data
 - Consults with research groups about their data management challenges
 - Develops and runs software, data, and author carpentry programming workshops
 - Implemented virtual reality workstation
- Graduate Research Assistant**, Princeton University, Princeton, NJ Jul. 2010-Jul. 2016
- Supervisor: Haw Yang
 - Initiated first computational work in group for interpreting single molecule fluorescence data
 - Developed Python software to automatically add fluorescence labeling points to proteins
 - Determined regulatory schemes for Protein Tyrosine Phosphatase B in *M. Tuberculosis*
 - Created data analysis methods for extracting motion in Insulin Degrading Enzyme
 - Simulated and discovered new conformations of Gramicidin S synthase A
- Graduate Teaching Assistant**, Princeton University, Princeton, NJ Sept. 2010-May 2011
- Taught 3 recitations for general chemistry, mentored students in advanced experiments
 - Designed recitation worksheets, held office hours, graded exams
 - Ran laboratories for upper-level students, graded reports; designed and led independent projects
 - Published independent project with students in the *Journal of Chemical Education*

Education

- Master of the Arts, Chemistry** Jan. 2012
Princeton University, Princeton, NJ
- Advisor: Professor Haw Yang
- Bachelor of the Arts, Chemistry, cum laude**, honors in major Jun. 2010
Hamilton College, Clinton, NY
- Minor: Physics

Publications

7. **Morrell, T. E.**; Rafalska-Metcalf, I. U.; Yang, H.; Chu, J-W. "Compound Molecular Logic in Accessing the Active Site of Mycobacterium tuberculosis Protein Tyrosine Phosphatase B" *J. Am. Chem. Soc.* **2018**, [10.1021/jacs.8b08070](https://doi.org/10.1021/jacs.8b08070)
6. Alfermann, J.; Sun, Xun; Mayerthaler, F.; **Morrell, T. E.**; Dehling, E.; Volkmann, G.; Komatsuzaki, T.; Yang, H.; Mootz, H. D. "FRET monitoring of a nonribosomal peptide synthetase" *Nat. Chem. Bio.* **2017**, [10.1038/nchembio.2435](https://doi.org/10.1038/nchembio.2435)
5. Sun, X.; **Morrell, T. E.**; Yang, H. "Extraction of Protein Conformational Modes from Distance Distributions Using Structurally Imputed Bayesian Data Augmentation" *J. Phys. Chem. B* **2016**, *120*, 10469-10482. [10.1021/acs.jpcc.6b07767](https://doi.org/10.1021/acs.jpcc.6b07767)
4. Landry, M. L.; **Morrell, T. E.**; Karagounis, T. K.; Hsia, C. -H.; Wang, C. -Y. "Simple Synthesis of CdSe Quantum Dots" *J. Chem. Educ.* **2014**, *91*, 274. [10.1021/ed300568e](https://doi.org/10.1021/ed300568e)
3. Temelso, B.; **Morrell, T. E.**; Shields, R. M.; Allodi, M. A.; Wood, E. K.; Kirschner, K. N.; Castonguay, T. C.; Archer, K. A.; Shields, G. C. "Quantum Mechanical Study of Sulfuric Acid Hydration: Atmospheric Implications" *J. Phys. Chem. A* **2012**, *116*, 2209. [10.1021/jp2119026](https://doi.org/10.1021/jp2119026)
2. Shields, R. M.; Temelso, B.; Archer, K. A.; **Morrell, T. E.**; Shields, G. C. "Accurate Predictions of Water Cluster Formation, (H₂O)_{n=2-10}" *J. Phys. Chem. A* **2010**, *114*, 11725. [10.1021/jp104865w](https://doi.org/10.1021/jp104865w)

1. **Morrell, T. E.**; Shields, G. C. "Atmospheric Implications for Formation of Clusters of Ammonium and 1-10 Water Molecules" *J. Phys. Chem. A* **2010**, *114*, 4266. [10.1021/jp911493](https://doi.org/10.1021/jp911493)

Selected Posters/Presentations

- RDA Plenary**, "Supporting Custom Data Services within an Institutional Data Repository" Philadelphia, Pennsylvania, April 2, 2019. [Poster](#)
- BE/Bi 103**, invited guest speaker "Research Data Management: Simple Ways to Make your Research Life Easier" Data Analysis in the Biological Sciences, Caltech, October 10, 2018. [Presentation](#)
- PEARC**, "Library and Research Computing Efforts and Tools to Improve Data Sharing and Archiving" Pittsburgh, Pennsylvania, June 24, 2018. Workshop + [Presentation](#)
- Open Repositories**, "Positioning a repository as campus research infrastructure" Bozeman, Montana, June 5, 2018. [Presentation](#)
- BE/Bi 103**, invited guest speaker "Research Data Management: Simple Ways to Make your Research Life Easier" Data Analysis in the Biological Sciences, Caltech, November 22, 2017. [Presentation](#)
- Open Repositories**, "Launching a Researcher-Focused Data Repository at Caltech using the Invenio 3 platform" Brisbane, Australia, June 25, 2017. [Presentation](#)
- Open Repositories**, "Building an open platform across diverse content and technologies" Brisbane, Australia, June 26, 2017. [Presentation](#)
- BE/Bi/NB 203**, invited guest speaker "Research Data Management: Simple Ways to Make your Research Life Easier" Introduction to Programming for the Biological Sciences Bootcamp, Caltech, June 22, 2017. [Presentation](#)
- American Chemical Society National Meeting**, Invited speaker for the Symposium in Honor of George C. Shields, Denver, CO, Mar. 23, 2015.
- American Chemical Society National Meeting**, "Allosteric coupling of correlated local unfolding and large-amplitude conformational change in proteins." Indianapolis, IN, Sept. 11, 2013.

Selected Instruction

- Software/Data Carpentry Python for postdocs**, Caltech, January 22-23; 29-30, 2019.
- Software Carpentry Git/Command Line for postdocs**, Caltech, November 13-14, 2018.
- Author Carpentry**, Caltech, October 25-26, 2018.
- Software Carpentry**, Caltech, August 13-16, 2018.
- Author Carpentry**, Wrote content and taught reproducible reporting using Rstudio. Force11 Scholarly Communications Institute, University of California, San Diego, July 30- August 3, 2018.
- Software/Data Carpentry Python for postdocs**, Caltech, May 7-8; 14-15, 2018.
- Software Carpentry Git**, Caltech, November 16, 2017.
- Author Carpentry**, Wrote content on sharing data and taught sharing data and publishing web content with GitHub. Force11 Scholarly Communications Institute, University of California, San Diego, August 2-3, 2017.
- Data Carpentry/GitHub Desktop**, Customized content to use GitHub Desktop and taught version control with git. Caltech, July 20-21, 2017.
- Data Carpentry for Humanists**, Customized content for audience and taught command line, git, and python sections. Caltech, May 6-7, 2017.
- Data Carpentry for Graduate Students**, Caltech, April 26-27, 2017.

Honors

- 2nd prize, Research Poster Competition, Princeton University Oct. 2013
- Pickering Teaching Award, Princeton University Jun. 2012
- Hugh Scott Taylor Prize, Physical Chemistry, Princeton University Sept. 2010
- NSF Graduate Research Fellowship 2010
- Donald J. Denney Prize in Physical Chemistry, Hamilton College Jun. 2010
- Norton Prize for Chemistry Research, Hamilton College Jun. 2010
- Elihu Root Fellowship to Pursue Graduate Work, Hamilton College Jun. 2010
- Sigma Xi Chemistry Honor Society Jun. 2010
- ACS/IREU Scholar May 2009