

Makenzie Long

Assistant Professor
Department of Chemistry
University of Central Arkansas

Education

Ph.D. in Physical Chemistry June 2014

University of Minnesota (Minneapolis, MN)

Advisor: Jiali Gao

Dissertation: "Insights into Proton-Coupled Electron Transfer from Computation"

B.S. in Chemistry May 2009

Kansas State University (Manhattan, KS)

Advisor: Christine Aikens

Thesis: "Adsorption of Formate on Gold Nanoparticles"

Experience

Assistant Professor August 2017 - Present

Department of Chemistry, University of Central Arkansas (Conway, AR)

Teaching: Undergraduate General Chemistry I

Undergraduate Physical Chemistry I (Kinetics and Quantum Mechanics)

Research: Model DNA-metal ion interactions using classical molecular dynamics and density functional theory (DFT) with a polarizable continuum model (PCM).

Postdoctoral Scholar and Lecturer August 2014 – July 2017

School of Natural Sciences, University of California Merced (Merced, CA)

Teaching: Undergraduate Quantum Chemistry and Spectroscopy

Advisor: Christine Isborn

Research: Validated and benchmarked computational methods for computing absorption spectra and simulating charge transfer dynamics in the gas and condensed phases.

Graduate Research Assistant January 2010 - July 2014

Department of Chemistry, University of Minnesota (Minneapolis, MN)

Advisor: Jiali Gao

Research: Developed and applied multistate density functional theory (MSDFT) to proton-coupled electron transfer (PCET) and other charge transfer processes in biological and chemical systems.

Summer Research Assistant June 2009 - August 2009

Nanoscience Center, University of Jyväskylä (Jyväskylä, Finland)

Advisor: Hannu Hakkinen

Research: Computed the circular dichroism spectra of Au₂₈ nanoparticles using time-dependent density functional theory (TDDFT).

Undergraduate Research Assistant

January 2008 - May 2009

Department of Chemistry, Kansas State University (Manhattan, KS)

Advisor: Christine Aikens

Research: Applied *ab initio* computational methods to study ligand binding on gold nanoparticles and the inherent chirality of gold nanoparticles.

Awards and Honors

Wiley Computers in Chemistry Outstanding Postdoc Award, Am. Chemical Society April 2017

Chancellor's Postdoctoral Fellowship, University of California Merced August 2015 - May 2017

Doctoral Dissertation Fellowship, University of Minnesota September 2013 - May 2014

Academic Fellowships, Dept. of Chemistry, University of Minnesota September 2009 - May 2010

Publications

Provorse Long, M. R.; Isborn, C. M. Combining Explicit Quantum Solvent with a Polarizable Continuum Solvent Model. *J. Phys. Chem. B* **2017**, *121*, 10105-10117.Milanese, J. M.; **Provorse, M. R.**; Alameda, E.; Isborn, C. M. Convergence of Computed Aqueous Absorption Spectra with Explicit Quantum Mechanical Solvent. *J. Chem. Theory Comput.* **2017**, *13*, 2159-2171.**Provorse, M. R.**; Peev, T.; Xiong, C.; Isborn, C. M. Convergence of Excitation Energies in Mixed Quantum and Classical Solvent: Comparison of Continuum and Point Charge Models. *J. Phys. Chem. B* **2016**, *120*, 12148-12159.Ren, H.; **Provorse, M. R.**; Bao, P.; Qu, Z.; Gao, J. Multistate Density Functional Theory for Effective Diabatic Electronic Coupling. *J. Phys. Chem. Lett.* **2016**, *7*, 2286-2293.**Provorse, M. R.**; Isborn, C. M. Electron Dynamics from Real-Time Time-Dependent Density Functional Theory. *Int. J. Quant. Chem.* **2016**, *116*, 739-749.**Provorse, M. R.**; Habenicht, B. F.; Isborn, C. M. Peak-Shifting in Real-Time Time-Dependent Density Functional Theory. *J. Chem. Theory Comput.* **2015**, *11*, 4791-4802.Habenicht, B. F.; Tani, N. P.; **Provorse, M. R.**; Isborn, C. M. Two-Electron Rabi Oscillations in Real-Time Time-Dependent Density-Functional Theory. *J. Chem. Phys.* **2014**, *141*, 184112.Gao, J.; Wang, Y.; Mazack, M. J. M.; Löffler, P.; **Provorse, M. R.**; Rehak, P. Explicit Polarization: A Quantum Mechanical Framework for Developing Next Generation Force Fields. *Acc. Chem. Res.* **2014**, *47*, 2837-2845.Chan, W.-L.; Berkelback, T. C.; **Provorse, M. R.**; Monahan, N. R.; Tritsch, J. R.; Hybertsen, M. S.; Reichman, D. R.; Gao, J.; Zhu, X.-Y. Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. *Acc. Chem. Res.* **2013**, *46*, 1321-1329.

Cembran, A.; **Provorse, M. R.**; Wang, C.; Wu, W.; Gao, J. The Third Dimension of a More O'Ferrall-Jencks Diagram for Hydrogen Atom Transfer in the Isoelectronic Hydrogen Exchange Reactions of $(\text{PhX})_2\text{H}\bullet$ with $\text{X} = \text{O}, \text{NH},$ and CH_2 . *J. Chem. Theory Comput.* **2012**, *8*, 4347-4358.

Hull, J.; **Provorse, M.**; Aikens, C. Formyloxyl Radical-Gold Nanoparticle Binding: A Theoretical Study. *J. Phys. Chem. A* **2012**, *116*, 5445-5452.

Provorse, M.; Aikens, C. Binding of Carboxylates to Gold Nanoparticles: A Theoretical Study of the Adsorption of Formate on Au_{20} . *Comp. Theor. Chem.* **2012**, *987*, 16-21.

Provorse, M.; Aikens, C. Origin of Intense Chiroptical Effects in Undecagold Subnanometer Particles. *J. Am. Chem. Soc.* **2010**, *132*, 1302-1310.

Research Presentations

Oral Presentations

"Convergence of Ground and Excited State Properties in the Condensed Phase" August 2016
252nd American Chemical Society National Meeting and Exposition (Philadelphia, PA)
Division of Computers in Chemistry: Quantum Chemistry

"Peak-Shifting in Real-Time Time-Dependent Density Functional Theory" October 2015
2015 American Chemical Society Midwest Regional Meeting (St. Joseph, MO)
Division of Physical Chemistry: Advances in Computational Chemistry

"Modeling Excited State Chemistry: Linear-Response and Real-Time Time-Dependent Density Functional Theory" October 2015
Physical Chemistry Seminar, Kansas State University (Manhattan, KS)

"Origin of Peak-Shifting in Real-Time Time-Dependent Density Functional Theory" March 2015
249th American Chemical Society National Meeting and Exposition (Denver, CO)
Division of Computers in Chemistry: Symposium Organizer Selections

"Insights into Proton-Coupled Electron Transfer from Multistate Density Functional Theory" October 2014
Chemistry and Chemical Biology Seminar, University of California Merced (Merced, CA)

"Multistate Density Functional Theory for Simulation of Enzymatic Reactions" August 2014
248th American Chemical Society National Meeting and Exposition (San Francisco, CA)
Division of Physical Chemistry: The Future of Computational Chemistry

"Quantum Coherence in Singlet Fission from Multistate Density Functional Theory" April 2013
Chemical Theory Center Seminar Series, University of Minnesota (Minneapolis, MN)

"Insights into Proton-Coupled Electron Transfer" May 2012
Graduate Student Research Symposium, University of Minnesota (Minneapolis, MN)

"Theoretical Study of the Adsorption of Formate on Au_{20} " November 2008
Kansas State University/University of Kansas Physical Chemistry Symposium (Manhattan, KS)

Poster Presentations

- "Towards a Better Understanding of Ion Mediated DNA-Surface Interactions: Transition and Alkaline Earth Metal Ion Interactions with a DNA Duplex" March 2018
255th American Chemical Society National Meeting and Exposition (New Orleans, LA)
Sci-Mix, Division of Physical Chemistry
- "Electronic Transitions in the Condensed Phase: Real-Time and Linear-Response Time-Dependent Density Functional Theory" April 2017
253rd American Chemical Society National Meeting and Exposition (San Francisco, CA)
Division of Computers in Chemistry: Wiley Computers in Chemistry Outstanding Postdoc Award
- "Insights into Proton-Coupled Electron Transfer from Computation" July 2014
Gordon Research Conference on Computational Chemistry (Mount Snow, VT)
- "Unraveling Free Radical Transport in Ribonucleotide Reductase" April 2014
2014 Doctoral Research Showcase, University of Minnesota (Minneapolis, MN)
- "Mechanism and Solvent Effects on Kinetic Isotope Effects for the Hydrogen Atom Abstraction of Ascorbic Acid by TEMPO Radical" May 2013
Chemistry Biology Interface Training Grant Symposium, University of Minnesota (Minneapolis, MN)
- "Quantum Coherence in Singlet Fission from Multistate Density Functional Theory" April 2013
Minnesota Supercomputing Institute Research Exhibition (Minneapolis, MN)
- "Insights into Proton-Coupled Electron Transfer" May 2012
Chemistry Biology Interface Training Grant Symposium, University of Minnesota (Minneapolis, MN)
- "Distinguishing Features between Proton-Coupled Electron Transfer and Hydrogen Atom Transfer from Multistate DFT" July 2011
World Association of Theoretical and Computational Chemists (Santiago de Compostela, Spain)
- "Theoretical Study of the Adsorption of Formate on Au₂₀" July 2008
American Conference on Theoretical Chemistry (Evanston, IL)

Additional Training**Teaching**

- The POGIL Project - Rocky Mountain (Southwest) Regional Meeting July 2015; June 16
Three-day workshop at Westminster College (Salt Lake City, UT); Santa Clara University (Santa Clara, CA)
- Teaching Matters Certificate Series
- Surviving the Classroom with 1st Generation College Students August 2014
- Developing Teaching Strategies September 2014
- One-day certificate practicums offered by the Center for Engaged Teaching and Learning at the University of California Merced (Merced, CA)

Graduate Student Workshop Facilitator

October 2011 - December 2011

Department of Chemistry, University of Minnesota (Minneapolis, MN)

Lead a workshop for chemistry undergraduate students on future career paths, what to consider when choosing a graduate program, and how to be successful in graduate school.

Poster Session Judge

October 2011

Undergraduate Research Conference, Council on Undergraduate Research, North Hennepin Community College (Brooklyn Park, MN)

Judged an undergraduate research poster session designed to encourage successful students to continue research at local four-year institutions.

Professional Memberships

American Chemical Society (ACS)

November 2013 - Present

Women in Science, Technology, Engineering, and Math (STEM)

September 2014 - July 2017

Sigma Alpha Epsilon - Xi Chapter/Graduate Women in Science

September 2010 - August 2011

Graduate and Professional Student Association (GAPSA)

September 2009 - May 2014

Council of Graduate Students (COGS)

September 2009 - May 2014

Women in Science and Engineering (WISE)

September 2005 - May 2014