

Mona Minkara

Kolthoff Hall, 225 Pleasant St. SE, Minneapolis, MN, 55455

☎ (781) 534-5831 • ✉ minka029@umn.edu • 🌐 www.monaminkara.com

Objective

To use my experience as a theoretical chemist to teach general, physical, and computational chemistry, while also applying what I've learned by researching computational biochemistry and interfacial physical chemistry to implement research projects that are both innovative and well-suited for undergraduates.

Education

University of Florida

Ph.D., Chemistry

Gainesville, FL

September 2011 – September 2015

Wellesley College

B.A., Chemistry and Middle-Eastern Studies

Wellesley, MA

September 2005 – September 2009

Awards & Honors

Dan Su Travel Award

The American Chemical Society Postdoc to Faculty Workshop

2018

Postdoctoral Scholar Travel Grant

MN Section of the American Chemical Society

2018

Postdoctoral Fellow Award

Penn Conference in Theoretical Chemistry

2017

Holman Prize Committee Member

Lighthouse

2017

Ford Foundation Postdoctoral Fellowship

National Academies of Sciences, Engineering, and Medicine

2016

NSF Graduate Research Fellowship

National Science Foundation

2012 – 2015

NFB Scholarship

National Federation of the Blind

2013

Alumni Fellowship

University of Florida

2010, '11, '12

Grinter Award

University of Florida

2010, '11, '12

Research Grant

Howard Hughes Medical Institute

2009, '10

Commencement Speaker

Wellesley College – [Click here to watch](#)

2009

National Scholastic Achievement Award

Learning Ally

2009

NSF Research Experiences for Undergraduates

National Science Foundation

2006, '07, '08, '09

Research Experience

University of Minnesota – Twin Cities

Postdoctoral Research Associate

Advisor: J. Ilja Siepmann

Minneapolis, MN

September 2015 – Present

Examining the effects of surfactants on the structural, transport, and thermodynamic properties of vapor bubbles in aqueous solutions.

Probing the miscibility gap of supercritical fluids.

Developing a new pressure equation of state for homo-oligomeric chains.

Elucidating fluid phase equilibria and structure of 2-dimensional surfactant monolayers.

Analyzing the adsorption of natural gas components at the water/gas interface and their effect on surface tension.

Studying loading of perfume raw materials into surfactant mesophases and the resulting structural changes.

University of Florida

National Science Foundation Graduate Research Fellow

Co-Advisors: Kenneth M. Merz Jr. & Erik Deumens

Dissertation: "Design of a Novel Inhibitor for *Helicobacter pylori*"

Gainesville, FL

September 2010 – September 2015

Discovered a new flap state in *Helicobacter pylori* urease (HPU) for the active site-covering flap.

Determined possible inhibitors for *Klebsiella aerogenes* urease, using docking study of over 14 million ligands from the ZINC database.

Discovered a possible pathway in which urea is shuttled into the active site of HPU.

Discovered, in conjunction with an exhaust flap, a possible pathway for the release of ammonium into surrounding environment.

Described my experience as a blind graduate student and published some of the methods that I used to conduct my research.

Wellesley College

Research Assistant

Advisor: Mala Radhakrishnan

Thesis: "Analyzing the Binding of Nevirapine and Rilpivirine to HIV-1 Reverse Transcriptase through Computationally Derived Charge Optimization"

Wellesley, MA

September 2007 – September 2010

Determined that rilpivirine's charge distribution was closest to optimal, resulting in a more effective drug.

Improved an electrostatics continuum model, boundary-integral based electrostatics estimation with interpolation.

Teaching Experience

Mentorship Program for Aspiring Chemistry Teachers (MPACT)

University of Minnesota

Minneapolis, MN

Spring 2018

Guest lectured twice for "Introduction to Quantum Mechanics and Spectroscopy" (CHEM4502) under mentorship by Professor Jason Goodpaster.

Preparing Future Faculty Course (GRAD8101)

University of Minnesota

Minneapolis, MN

Fall 2017

Learned about various teaching techniques and taught a lesson on *Teams, Groups, and Cooperative Learning*.

STEM Curriculum Instructor for Empowerment Through Integration*American University of Beirut***Beirut, Lebanon***Summers 2017, 2018*

Led a team on implementing a low-cost blind-accessible STEM curriculum taught to blind children ages 6 – 26.

Research project mentor to an undergraduate student*University of Minnesota***Minneapolis, MN***January 2017 – Present*

Published a first-authored manuscript written by the undergraduate, Colin Bunner: "Gibbs Ensemble Monte Carlo Simulations Probing the Miscibility Gap in Water/Hydrogen Mixtures at High Temperatures and Pressures."

Seminar Session Teacher*University of Minnesota***Minneapolis, MN***October 2016*

Prepared and taught a session for "Probing Chemical Systems with Molecular Simulation" (CHEM1905).

Research project mentor to a high school student*University of Minnesota***Minneapolis, MN***Summer 2016*

Published an article with the student, Daniel Stein: "Monte Carlo Simulations Probing the Liquid/Vapour Interface of Water/Hexane Mixtures: Adsorption Thermodynamics, Hydrophobic Effect, and Structural Analysis."

General Chemistry TA (CHM2045)*University of Florida***Gainesville, FL***Summer 2014*

Prepared and taught two recitation sections for the full semester.

Pforzheimer Learning & Teaching Center Tutor*Wellesley College***Wellesley, MA***September 2008 – September 2009*

Each semester, tutored undergraduate Mathematics and Arabic to and three to four permanent students plus drop-ins.

Publications

"Gibbs Ensemble Monte Carlo Simulations Probing the Miscibility Gap in Water/Hydrogen Mixtures at High Temperatures and Pressures." Bunner, C.E.; **Minkara, M.S.**; Siepmann, J.I. *J. Chem. Phys., in preparation*

"A New Equation of State for Homo-polymers in Dissipative Particle Dynamics." **Minkara, M.S.**; Hembree, R.H.; Jamadagni, S.N.; Ghobadi, A.F.; Eike, D.M.; Siepmann J.I. *Submitted to J. Chem. Phys.*

"Monte Carlo Simulations Probing the Liquid/Vapour Interface of Water/Hexane Mixtures: Adsorption Thermodynamics, Hydrophobic Effect, and Structural Analysis." **Minkara, M.S.**; Josephson, T.; Venteicher, C.L.; Chen, J.L.; Stein, D.J.; Peters, C.J.; Siepmann, J.I. *Mol. Phys.* **2018**, published online. DOI: 10.1080/00268976.2018.1471233

"Probing Additive Loading in the Lamellar Phase of a Nonionic Surfactant: Gibbs Ensemble Monte Carlo Simulations using the SDK Force Field." **Minkara, M.S.**; Lindsey, R.K.; Hembree, R.H.; Venteicher, C.L.; Jamadagni, S.N.; Eike, D.M.; Ghobadi, A.F.; Koenig, P.H.; Siepmann, J.I. *Langmuir* **2018**, published online. DOI: 10.1021/acs.langmuir.8b00687

"Reduction of Urease Activity by Interaction with the Flap Covering the Active Site." Macomber, L.; **Minkara, M.S.**; Hausinger, R.P.; Merz, K.M., Jr. *J. Chem. Inf. Model.* **2015**, DOI: 10.1021/ci500562t

"Implementation of Protocols to Enable Doctoral Training in Physical and Computational Chemistry of a Blind Graduate Student." **Minkara, M.S.**; Weaver, M.N.; Gorske, J.; Bowers, C.R.; Merz, K.M., Jr. *Chem. Educ.* **2015**, DOI: 10.1021/ed5009552

"Effect of 10.5 M Aqueous Urea on *Helicobacter pylori* Urease: A Molecular Dynamics Study." **Minkara, M.S.**; Weaver, M.N.; Merz, K.M., Jr. *Biochemistry* **2015**, DOI: 10.1021/acs.biochem.5b00078

"Molecular Dynamics Study of *Helicobacter pylori* Urease." **Minkara M.S.**; Ucisik, M.N.; Weaver, M.N.; Merz, K.M., Jr. *J. Chem. Theory Comput.* **2014**, DOI: 10.1021/ct5000023

"Analysis of fast boundary-integral approximations for modeling electrostatic contributions of molecular binding." Kreienkamp, A.B.; Liu, L.Y.; **Minkara, M.S.**; Knepley, M.G.; Bardhan, J.P.; Radhakrishnan, M.L. *Mol. Based Math. Biol.* **2013**, DOI: 10.2478/mlbmb-2013-0007

"Multiple drugs and multiple targets: An analysis of the electrostatic determinants of binding between non-nucleoside HIV-1 reverse transcriptase inhibitors and variants of HIV-1 RT." **Minkara, M.S.**; Davis, P.H.; Radhakrishnan, M.L. *Proteins* **2012**, DOI: 10.1002/prot.23221

Invited Talks

"Probing Interfaces and Mesophases with Molecular Simulation." Northeastern University, Boston, MA, August 2018.

"Navigating Graduate School with a Disability." University of California, Berkeley, CA, April 2018.

"Probing Interfaces and Mesophases with Molecular Simulation." Michigan State University, East Lansing, MI, February 2018.

"A Computational Study of How Solutes Load into a Surfactant Bilayer Using Monte Carlo Techniques." Carleton College, Northfield, MN, February 2018.

"Journey of a Blind Computational Chemist." University of Arkansas, Fayetteville, AR, May 2017.

"Molecular Simulation Studies Aiding Drug Design and Delivery." Vanderbilt University, Nashville, TN, April 2017.

"Chemistry Through Blind Eyes." Universidad Iberoamericana, Mexico City, Mexico, October 2016.

"Molecular Dynamics Study of *Helicobacter pylori* Urease." Wellesley College, Wellesley, MA, February 2015.

"Molecular Dynamics Simulations Investigating *Helicobacter pylori* Urease." University of Minnesota, Minneapolis, MN, January 2015.

Conference Presentations

"Probing Curvature Effects on Surfactant Adsorption onto the Liquid/vapor Interfaces of Water Using Monte Carlo Simulations." 256th National Meeting of the American Chemical Society, Boston, MA, August 2018.

"Unseen Advantage: The Alternate Perspective of a Blind Computational Chemist." 256th National Meeting of the American Chemical Society, Boston, MA, August 2018.

"Adsorption of Hexane and H₂S at the Liquid-Vapor Interface of Water." Annual IPRIME meeting at the University of Minnesota, Minneapolis, MN, June 2018. *Click here to watch*

"Gibbs ensemble Monte Carlo Simulations for Additive Loading in Surfactant Bilayers." 255th National Meeting of the American Chemical Society, New Orleans, LA, March 2018.

"Gibbs ensemble Monte Carlo Simulations for Additive Loading in Surfactant Bilayers." 2017 Penn Conference in Theoretical Chemistry, Philadelphia, PA, August 2017.

"Tools of a Blind Chemist." 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2017.

"Monte Carlo Simulations Probing the Liquid/Vapor Interface of Water/Hexane Mixtures." 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2017.

"Chemistry Through Blind Eyes." Plenary lecture at the International Symposium on the Teaching of Sciences to Visually Impaired People, at the Normal School for Teachers: Moisés Sáenz, Monterrey, Mexico, September 2016.

"Probing Vapor-liquid Equilibria of Pentadecanoic Acid Langmuir Monolayers." Annual IPRIME meeting at the University of Minnesota, Minneapolis, MN, June 2016.

"Probing Vapor-liquid Equilibria of Pentadecanoic Acid Langmuir Monolayers." Midwest Thermodynamics and Statistical Mechanics Conference at Miami University, Oxford, OH, May 2016.

"Using Access Technologies in the Chemistry and Science Laboratory Classrooms for Multi-Sensory Data Acquisition." 247th National Meeting of the American Chemical Society, Dallas, TX, March 2014.

Posters.....

"Probing Curvature Effects on Surfactant Adsorption onto the Liquid/vapor Interfaces of Water Using Monte Carlo Simulations." **Minkara, M.S.** & Siepmann, J.I. 256th National Meeting of the American Chemical Society, Boston, MA, August 2018.

"Probing Mesophases and Interfaces using Monte Carlo Simulations." **Minkara, M.S.** & Siepmann, J.I. 256th National Meeting of the American Chemical Society, Boston, MA, August 2018.

"Liquid-Liquid and Liquid-Vapor Interfacial Tension and Preferential Adsorption for Water/Oil Mixtures." **Minkara, M.S.**; Chen, J.L.; Siepmann, J.I. IPRIME 2017 Annual Meeting, Minneapolis, MN, June 2017.

"Vapor-Liquid and Liquid-Liquid Equilibria for a Langmuir Monolayer of Pentadecanoic Acid: A Monte Carlo Study." **Minkara, M.S.** 253rd National Meeting of the American Chemical Society, San Francisco, CA, April 2017.

"Monte Carlo Studies of Vapor-Liquid Equilibria for a Langmuir Monolayer of Pentadecanoic Acid." **Minkara, M.S.**; Lindsey, R.K.; Siepmann, J.I. 251st National Meeting of the American Chemical Society, San Diego, CA, March 2016.

"Probing Electrostatic Interactions between Amino Acids and Urea using *ab initio* Calculations." **Minkara, M.S.**; Urul, D.A.; Weaver, M.N.; Merz, K.M., Jr. 251st National Meeting of the American Chemical Society, San Diego, CA, March 2016.

"Molecular Dynamics Study of *Helicobacter pylori* Urease in 150 Millimolar Aqueous NH₄Cl." **Minkara, M.S.**; Weaver, M.N.; Merz, K.M., Jr. 249th National Meeting of the American Chemical Society, Denver, CO, March 2015.

"Effect of 10.5 M Aqueous Urea on *Helicobacter pylori* Urease: A Molecular Dynamics Study." **Minkara, M.S.**; Weaver, M.N.; Merz, K.M., Jr. 248th National Meeting of the American Chemical Society, San Francisco, CA, August 2014.

"Molecular Dynamics Study of *Helicobacter pylori* Urease." **Minkara, M.S.**; Ucisik, M.N.; Weaver, M.N.; Merz, K.M., Jr. 247th National Meeting of the American Chemical Society, Dallas, TX, March 2014.

"A Computational Analysis of Molecular Recognition in the Trypsin/Bovine Pancreatic Trypsin Inhibitor (BPTI) System Using Multiple Electrostatic Models." **Minkara, M.S.**; Bardham, J.; Radhakrishnan, M.L. The Protein Society 24th Annual Symposium, San Diego, CA. August 2010.

"Improving the Binding of Nevirapine and Rilpivirine to HIV-1 Reverse Transcriptase through Computationally Derived Charge Optimization." **Minkara, M.S.** & Radhakrishnan, M.L. Senior Research Thesis, Department of Chemistry, Wellesley College, Wellesley, MA, April 2009.

"Analyzing Electrostatic Determinants of Affinity and Promiscuity in the HIV-1 Reverse Transcriptase." **Minkara, M.S.** & Radhakrishnan, M.L. Presented at the 53rd Annual meeting of the Biophysical Society, Boston, MA, March 2009.

"Improving the Binding of Nevirapine and Rilpivirine to HIV-1 Reverse Transcriptase through Computationally Derived Charge Optimization." **Minkara, M.S.** & Radhakrishnan, M.L. Presented at the 237th National Meeting of the American Chemical Society, Salt Lake City, UT, March 2009.

Outreach

STEM Curriculum Coordinator/Developer for Empowerment Through Integration **Beirut, Lebanon**
American University of Beirut *Summers 2017, 2018*

Led a team on designing/implementing a low-cost blind-accessible STEM curriculum for blind children ages 6 – 26.

Guest Presenter **Minneapolis, MN**
Washburn High School *November 2017*

Presented a talk titled "Journey of a Blind Computational Chemist"

Guest Presenter **Minneapolis, MN**
University of Minnesota Chemistry Section of Women in Science and Engineering *September 2017*

Presented a talk titled "Journey of a Blind Computational Chemist"

Guest Presenter **Minneapolis, MN**
Wellstone International High School *May 2017*

Presented a talk titled "Journey of a Blind Computational Chemist"

Guest Presenter **Minneapolis, MN**
Thomas Edison High School *May 2017*

Presented a talk titled "Journey of a Blind Computational Chemist"

Guest Presenter **Minneapolis, MN**
University of Minnesota student group, Girls Rising *May 2017*

Presented a talk titled "Journey of a Blind Computational Chemist"

Professional Affiliations

ACS Chemists with Disabilities Committee
Associate *2017 – Present*

National Federation of the Blind
Member *2011 – Present*

American Chemical Society
Member *2008 – Present*

References

J. Ilja Siepmann
Postdoctoral Advisor
Address: 207 Pleasant St. SE
Minneapolis, MN 55455
Phone: (612) 624-1844
Email: siepmann@umn.edu

Kenneth M. Merz Jr.
Graduate Advisor
Address: 578 S Shaw Ln.
East Lansing, MI 48824
Phone: (517) 355-9715
Email: kmerz1@gmail.com

Mala Radhakrishnan
Undergraduate Advisor
Address: 106 Central Street
Wellesley, MA 02481
Phone: (781) 283-2981
Email: mradhakr@wellesley.edu

Jason Goodpaster
MPACT Mentor
Address: 207 Pleasant St. SE
Minneapolis, MN 55455
Phone: (612) 624-8825
Email: jgoodpas@umn.edu