CURRICULUM VITAE

DANIELA KOHEN

Chemistry Department
Carleton College
Northfield, MN 55057

(507) 645-4598 (H)
(507) 222-7165 (W)

dkohen@carleton.edu

EDUCATION

Doctor in Philosophy, Chemical Physics, University of Notre Dame.
Thesis title: "Phase Space Distribution Function Approach to Molecular Dynamics in Solution." Advisor: David J. Tannor. 1995.

Bachelor of Arts, Chemistry Major. Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Argentina. 1990.

TEACHING EXPERIENCE

Carleton College, Chemistry Department. Professor. General Chemistry, Quantum Chemistry, Chemical Thermodynamics, Statistical Thermodynamics, Advanced Kinetics Laboratory, Computational Chemistry, Time Dependent Quantum Mechanics, The Integrative Exercise (Comps). January, 2002-present.

Smith College, Chemistry Department. Visiting Assistant Professor. General Chemistry, Physical Chemistry of Biochemical Systems, and Physical Chemistry Laboratory. August, 1999-December, 2002.

University of Notre Dame, Chemistry Department. Teaching Assistant. General Chemistry Laboratory. Fall 1990.

Universidad de Buenos Aires, Departmento de Química Inorgánica, Analítica y Físico-Química. Undergraduate teaching assistant. General Chemistry, Inorganic Chemistry and Physical Chemistry. 1988-1990.

Universidad de Buenos Aires. Undergraduate teaching assistant. General Chemistry Introductory Courses. 1987-1988.

RESEARCH EXPERIENCE

University of California, Irvine, Chemistry Department. Post Doctoral Fellow. Supervisor: Craig C. Martens. 1998-1999.

Lucent Technologies, Bell Labs Innovations, Material Chemistry Research Department. Post Doctoral Member of Technical Staff. Supervisors: Frank H. Stillinger and John C. Tully. 1995-1997.

University of Notre Dame, Chemistry Department. Research Assistant. Advisor: David J. Tannor. 1991-1995.

Universidad de Buenos Aires, Departmento de Química Inorgánica, Analítica y Físico-Química. Undergraduate Research Assistant. Advisor: Miguel Blesa. 1988-1990.

ARTICLES (underlined names correspond to undergraduates)

1. "Molecular Insight into CO_2 "Trapdoor" Adsorption in Zeolite Na-RHO." Chemistry of Materials, **29**, 2724 (2017). François-Xavier Coudert and Daniela Kohen.

2. "Theoretical Mechanistic Study of the Asymmetric Desymmetrization of a Cyclic meso-Anhydride by a Bifunctional Quinine Sulfonamide Organocatalyst." J. Org. Chem., **82**, 1347 (2017). Katie Blise, Milan W. Cvitkovic, Nolly J. Gibbs, Sean F. Roberts, Reid M. Whitaker, Gretchen E. Hofmeister, and Daniela Kohen.

3. "Computational Chemistry Methods for Nanoporous Materials." Chemistry of Materials, **29**, 199 (2016). Jack D Evans, Guillaume Fraux, Romain Gaillac, Daniela Kohen, Fabien Trousselet, Jean-Mathieu Vanson, and François-Xavier Coudert.

4. "Atomistic Simulations of CO_2 during "Trapdoor" Adsorption onto Na-Rho Zeolite". Foundations of Molecular Modeling and Simulation: Select Papers from FOMMS 2015; Springer: 2015, 153. N. Bamberger, D. Kohen.

5. "A computational study of the adsorption of n-perfluorohexane in zeolite BCR-704." Fluid Phase Equil., **366**, 146 (2014). P. Bai, P. Ghosh, J. Sung, D. Kohen, J.I. Siepmann, and R.Q. Snurr.

6. "Development of a Regional Computational Chemistry Consortium Centered around Undergraduate Research Conferences.", CUR Quarterly 2012, 329 (2012). Keith T. Kuwata, Daniela Kohen, Brent P. Krueger, and William F. Polik.

7. "Atomistic Simulations of CO_2 and N_2 within Cage Type Silica Zeolites." Langmuir, **27**, 1954 (2011). Lindsey Madison, Henry Heitzer, Colin Russell and Daniela Kohen. (This paper was showcased as a paper of the week by the ACS web portal)

8. "Atomistic Simulations of CO_2 and N_2 Diffusion in Silica Zeolites: The Impact of Pore Size and Shape." J. Phys. Chem. C, **112**, 16521 (2008). David Selassie, Disan Davis, Jayme Dahlin, Eric Feise, David S. Sholl and Daniela Kohen.

9. "Atomistic Simulations of CO_2 and N_2 adsorption in Silica Zeolites: The impact of pore size and shape." J. Phys. Chem. B, **106**, 8367 (2002). A. Goj, D. S. Sholl, E. D. Akten and D. Kohen.

10. "The manipulation of massive ro-vibronic superpositions using time-frequency-resolved coherent anti-Stokes Raman scattering (TFRCARS): from quantum coherence to quantum computing." Chem. Phys., **266,** 323 (2001). R. Zadoyan, D. Kohen and V. A. Apkarian.

11. "Simulation of nonadiabatic wavepacket interferometry using classical trajectories." J. Chem. Phys., **112,** 7345 (2000). A. Donoso, D. Kohen and C. C. Martens.

12. "Diversity in liquid supercooling and glass formation phenomena illustrated by a simple model." Physical Review E **61,** 1176 (2000). D. Kohen and F. H. Stillinger.

13. "Phase space approach to dissipative molecular dynamics." Advances in Chemical Physics **111,** 219 (2000). D. Kohen and D. J. Tannor.

14. "Nanoscale shock wave spectroscopy: a direct view of coherent ultrafast bath dynamics." J. Phys. Chem., **111,** 4343 (1999). D. Kohen and C. C. Martens.

15. "Model studies of non-adiabatic dynamics." J. Chem. Phys., **109**, 4713 (1998). D. Kohen, F. H. Stillinger and J. C. Tully.

16. "Modeling the interactions of hydrogen with silicon surfaces." Surface Science, **397**, 225 (1998). D. Kohen, J. C. Tully and F. H. Stillinger.

17. "Classical-quantum correspondence in the Redfield equation and its solutions." J. Chem. Phys., **107**, 5141 (1997). D. Kohen and D. J. Tannor.

18. "Phase space approach to theories of quantum dissipation." J. Chem. Phys., **107**, 5236 (1997). D. Kohen, C. C. Marston and D. J. Tannor.

19. "Phase space distribution function formulation of the method of reactive flux: memory friction." J. Chem. Phys. **103**, 6013 (1995). D. Kohen and D. J. Tannor.

20. "Derivation of Kramers' formula for condensed phase reaction rates using the method of reactive flux." J. Chem. Phys. **100**, 4932 (1994). D. Kohen and D. J. Tannor.

21. "Quantum adiabatic switching." J. Chem. Phys. **98**, 3168 (1993). D. Kohen and D. J. Tannor.

AWARDS

- "Acquisition of a High Performance Computing Cluster for Undergraduate Chemistry Research and Teaching by the Midwest Undergraduate Computational Chemistry Consortium (MU3C)" Granted by NSF-MRI. August 2019. $400,400.

- "RUI: Molecular Insight into Cation Motion within Zeolites". Granted by NSF. May 2019. $183,416.

- "Atomistic Simulations of Small Molecules' Behavior within Al Substituted Zeolites." Granted by PRF. January 2012.

- "MRI: Acquisition of a Computer Cluster for Undergraduate Chemistry Research and Teaching by the Midwest Undergraduate Computational Chemistry Consortium (MU3C)." Granted by NSF-MRI. September 2010.

- "Studying the behavior of CO_2 within zeolites: atomistic simulations." Granted by PRF. June 2006.

- "Acquisition of a Computer Cluster for Research, Research Training, and Teaching." In collaboration with Hope, Macalester, and Gustavous Adolphus Colleges. Granted by NSF-MRI. August 2005.

- "Introducing Theoretical and Computational Chemistry to Carleton College." Faculty Start-up Grant Program for Undergraduate Institutions; granted by the Camille and Henry Dreyfus Foundation. July 2002.

INVITED RESEARCH TALKS

- "Molecular Insight on the Behavior of Carbon Dioxide within Zeolites" Midwest Thermodynamics and Statistical Mechanics Conference, University of Notre Dame, IN. June 2017

- "Behavior of Carbon Dioxide within Zeolites: Atomistic Simulations" Foundations of Molecular Modeling and Simulation, Mt. Hood, OR. July 2015.

- "Atomistic simulations of CO_2 and N_2 within zeolites" Midwest Thermodynamics and Statistical Mechanics Conference, Wheaton College, IL. June 2011

- "Atomistic simulations of CO_2 and N_2 within zeolites." Fall ACS meeting, Symposium Title: Surface Chemistry and Environmental Applications of Nanoporous Materials. Boston, MA. August 2010.

- "Studying carbon dioxide in zeolites: Atomistic simulations." Gustavus Adolphus College, MN. April 2008.

- "Studying carbon dioxide in zeolites: Atomistic simulations." Northwestern University, IL. April 2007.

- "Studying carbon dioxide in zeolites: Atomistic simulations." University of Madison, WI. March 2007.

- "Studying carbon dioxide in zeolites: Atomistic simulations." Grinnell College, Grinnell IA. February 2007.

- "Studying carbon dioxide in zeolites: Atomistic simulations." St. Olaf College, Northfield MN. September 2006.

- "Studying carbon dioxide in zeolites: Atomistic simulations." University of Iowa, Iowa City, IA. November 2005.

RESEARCH CONFERENCE PRESENTATIONS (* names correspond to presenters)

- "Molecular insight into cation motion within zeolites". D. Kohen*. Talk. Thirteen Fundamentals of Adsorption Conference. Cairns, Australia. May 2019.
- "Cation Behavior within Zeolites" A. Nijhawan*, B. Lynch, and D. Kohen. Poster. ACS, Orlando Fl, March 2019. This poster won the "Recognition for Outstanding Research" award.
- "Structure and Reactivity in Ruthenium Silyl and Silylene Complexes: a Computational Study". W. deSnoo*, M. Whited, and D. Kohen. Poster. ACS, Orlando Fl, March 2019.
- "Synthetic and Computational Investigation of Cobalt Silylene Reactivity". A. Conley*, Jim Zhang*, M. Whited, and D. Kohen. Poster. ACS, Orlando Fl, March 2019.
- "Sodium Cation Behavior within Zeolites." Adam Nijhawan* and Brody Lynch*. Poster. Scholars at the Capitol Event, St. Paul, MN. January 2019.
- "Cation Motions within Zeolites: A Molecular Dynamics Study." Adam Nijhawan* and Brody Lynch*. Talk. Thirty-First Midwest Undergraduate Computational Chemistry Symposium, University of Minnesota, Twin Cities. July 2018.
- "Structure and Bonding in Ruthenium Silyl and Silylene Complexes." Will deSnoo*. Talk. Thirty-First Midwest Undergraduate Computational Chemistry Symposium, University of Minnesota, Twin Cities. July 2018.
- "Molecular insight into CO_2 "Trapdoor" Adsorption in zeolite Rho. " Adam Nijhawan, Brody Lynch, FX Coudert, and Daniela Kohen*. Poster. 8th International Workshop on Characterization of Porous Delray Beach, Fl. May 2018.

- "Can Transition State Analogues be Used to Predict Enantioselectivity?" Elianna Frank*, Daniela Kohen and Gretchen Hofmeister. Poster. ACS, New Orleans, March 2018. This poster won the "Outstanding Research Jeffrey Madura Award."
- "Molecular insight into CO_2 "Trapdoor" Adsorption in zeolite Rho. " Adam Nijhawen, Brody Lynch, FX Coudert, and Daniela Kohen*. Poster. Gordon Research Conference, Andover, NH. August 2017
- "Can Transition State Analogues be Used to Predict Enantioselectivity?" Elianna Frank*. Talk. Twenty-Nith Midwest Undergraduate Computational Chemistry Symposium, University of Illinois, Urbana-Champaign. July 2017.
- "Cation Motions within Zeolites: A Molecular Dynamics Study." Adam Nijhawand and Brody Lynch*. Talk. Twenty-Nith Midwest Undergraduate Computational Chemistry Symposium, University of Illinois, Urbana-Champaign. July 2017.
- "Computational Examination of Structure and Bonding in Ruthenium Silyl and Silylene Complexes." Will deSnoo*. Poster. Twenty-Nith Midwest Undergraduate Computational Chemistry Symposium, University of Illinois, Urbana-Champaign. July 2017.
- "Molecular insight into CO_2 "Trapdoor" Adsorption in zeolite Rho." FX Coudert and Daniela Kohen*. Talk. Twelfth Fundamentals of Adsorption Conference. Lake Constance, Germany. June 2016.
- "Studying Carbon Dioxide in Zeolites: Atomistic Simulations ". Daniela Kohen*. Talk. Twenty-Fifth Midwest Undergraduate Computational Chemistry Symposium, Northwestern University, Evanston, IL. July 2015.
- "Employing Organocatalysts for Biorenewable Desymmetrization: A Quantum Mechanical Study". Katie Blise* Gretchen Hofmeister, Dave Alberg and Daniela Kohen. Poster. National ACS meeting, Denver, CO. March 2015. (This poster won the best poster award at its session)
- "Sodium and Carbon Dioxide Behavior within Al-Substituted Zeolites". Nathan Bamberger* and Kit Pavlekovsky*.Talk. Twenty-Third Midwest Undergraduate Computational Chemistry Symposium, Iowa State University, Ames, IA. July 2014.
- "Manipulating Strong Bonds through Transition metal-Element Cooperation: A DFT Study" Eliza Green*. Twenty-Third Midwest Undergraduate Computational Chemistry Symposium, Iowa State University, Ames, IA. July 2014.
- "Organocatalysts for Biorenewable Desymmetrization: A Quantum Mechanical Study". Katie Blise* Twenty-Third Midwest Undergraduate Computational Chemistry Symposium, Iowa State University, IA. July 2014.
- "Atomistic Simulations of CO_2 and N_2 within Zeolites". Nathan Bamberger, Kit Pavlekovsky, and Daniela Kohen*. Poster. Gordon Research Conference, Holderness, NH. August 2013.
- "Carbon Dioxide Behavior within Al-Substituted Zeolites" Nathan Bamberger* and Kit Pavlekovsky*. Talk. Twenty-First Midwest Undergraduate Computational Chemistry Symposium, University of Michigan, Ann Arbor, MI. July 2013.
- "Organocatalysts for Biorenewable Desymmetrization: A Quantum Mechanical Study." Katie Blise*. Talk. Twenty-First Midwest Undergraduate Computational Chemistry Symposium, University of Michigan, Ann Arbor, MI. July 2013.
- "Organocatalysts for biorenewable desymmetrization." Milan Cvitkovic*, Gretchen Hofmeister, Dave Alberg and Daniela Kohen. Poster. National ACS meeting, New Orleans, LA. March 2013.
- "Atomistic Simulations of CO_2 and N_2 within Zeolites" Katie Deeg, Diane Walters, Jie Lin, Annete Martin and Daniela Kohen*. Poster. FOMMS. Mt. Hood, Oregon, July 2012.
- "CO_2 adsorption in Al-Substituted Zeolites " Jie Lin* and Annette Martin*. Talk. Nineteen Midwest Undergraduate Computational Chemistry Symposium, University of Minnesota, Minneapolis, MN. July 2012.
- "Computational Investigations of Organocatalysts for Biorenewable Desymmetrization." Milan Cvitkovic* Talk. Nineteen Midwest Undergraduate Computational Chemistry Symposium, University of Minnesota, Minneapolis, MN. July 2012.
- "Atomistic Simulations of CO_2 and N_2 within Zeolites" Katie Deeg, Diane Walters and Daniela Kohen*. Poster. CPM-6. Del Rey Beach, Florida, April 2012.
- "CO_2 Preferential Adsorption Sites in MFI-Type Zeolites" Katie Deeg, Diane Walters and Daniela Kohen*. Poster. National ACS meeting, San Diego, CA. March 2012.
- The role of cations in the behavior of Carbon dioxide behavior within Aluminum substituted zeolites." Seventeen Midwest Undergraduate Computational Chemistry Symposium, University of Chicago. July 2011. Talk. Katie Deeg* and Diane Walters* and Daniela Kohen.
- "The role of cations in the behavior of carbon dioxide on zeolites." Fifteen Midwest Undergraduate Computational Chemistry Symposium, University of Madison-Wisconsin. July 2010. Talk. Katie Deeg* and Diane Walters* and Daniela Kohen.

- "Atomistic Simulations of CO_2 and N_2: Adsorption and Diffusion in Zeolites with cages connected by narrow pores." National ACS meeting, San Francisco, CA. March 2010. Poster. Henry Heitzer*, Lindsey Madison*, Colin Russell* and Daniela Kohen.
- "The role of rotation in the behavior of CO_2 within zeolites with cages." Eleventh Midwest Undergraduate Computational Chemistry Symposium, Northwestern University. July 2009. Talk. Lindsey Madison* and Daniela Kohen.
- "Exploring CO_2 and N_2 diffusion within the LTA zeolite." Eleventh Midwest Undergraduate Computational Chemistry Symposium, Northwestern University. July 2009. Talk. Henry Heitzer* and Daniela Kohen.
- "The role of Coulombic interactions in determining the behavior of CO_2 and N_2 within all-silica zeolites." Eleventh Midwest Undergraduate Computational Chemistry Symposium, Northwestern University. July 2009. Talk. Colin Russell* and Daniela Kohen.
- "Atomistic Simulations of CO_2 and N_2 in Silica Zeolites: The Impact of Pore Size and Shape." Foundations of Molecular Modeling and Simulations Conference. July 2009, Blaine, WA. Poster. Henry Heitzer*, Lindsey Madison*, Colin Russell*, and Daniela Kohen.
- "How do CO_2 and N_2 orient themselves within the ITQ-3 zeolite?" Mercury Conference on Computational Chemistry, Hamilton NY. July 2008. Poster. Lindsey Madison* and Daniela Kohen.
- "CO_2 and N_2 behavior within the LTA zeolite." Mercury Conference on Computational Chemistry, Hamilton NY. July 2008. Poster. Henry Heitzer* and Daniela Kohen.
- "Do Coulombic interactions dominate the rate of diffusion of CO_2 and N_2 within all-silica zeolites?" Mercury Conference on Computational Chemistry, Hamilton NY. July 2008. Poster. Colin Russell* and Daniela Kohen.
- "Atomistic Simulations of CO_2 and N_2 in Silica Zeolites: the impact of pore size and shape." ACTC Conference, Northwestern University, Evanston, IL. July 2008. Poster. David Selassie*, Anne Goj, David S. Sholl, Jayme Dahlin*, Disan Davis* and Daniela Kohen.
- "Atomistic Simulations of CO_2 and N_2 in Silica Zeolites: the impact of pore size and shape." Nanoporous Materials Gordon Research Conference. June 2008, Colby College, Waterville, ME. Poster. David Selassie, Anne Goj, David S. Sholl, Jayme Dahlin, Disan Davis and Daniela Kohen.
- "Atomistic Simulations of CO_2 and N_2 behavior in Zeolites" National ACS meeting. April 2008, New Orleans, LA. Poster. David Selassie*, Felix Amankona-Diawuo*, Dan Kemp, Lyuda Slipchenko and Daniela Kohen.
- "Atomistic Simulations of CO_2 and N_2 Adsorption and Diffusion in Zeolites." AIChE's Annual Meeting. November, 2007, Salt Lake City, UT. Talk. Daniela Kohen.
- "Carbon Dioxide and Nitrogen in Zeolites: Diffusion and Potential Energies." Sixth Midwest Undergraduate Computational Chemistry Symposium. August 2007, University of Illinois, Champaign-Urbana. Talk. David Selassie* and Daniela Kohen.
- "Using the Effective Fragment Potential in atomistic simulation of CO_2 adsorption in Zeolites." Sixth Midwest Undergraduate Computational Chemistry Symposium. August 2007, University of Illinois, Champaign-Urbana. Talk. Felix Amankona-Diawuo* and Daniela Kohen.
- "Computational Chemistry Investigations for Undergraduates." Chair and Organizer of the symposium at the National ACS Meeting, September 2006.
- "Analysis of Carbon Dioxide behavior in zeolites." Fourth Midwest Undergraduate Computational Chemistry Symposium. August 2006, Iowa State University. Talk. Felix Amankona-Diawuo,* David Selassie* and Daniela Kohen.
- "Analysis of of the preferred Sites of CO_2 and N_2 in silica zeolites." Fourth Midwest Undergraduate Computational Chemistry Symposium. August 2006, Iowa State University. Talk. Jayme Dahlin* and Daniela Kohen.
- "Studying CO_2 in Zeolites: Atomistic Simulations." Foundations of Molecular Modeling and Simulations Conference. July 2006, Blaine, WA. Poster. Disan Davis, Jayme Dahlin, Anne Goj and Daniela Kohen.*
- "Studying CO_2 in Zeolites: Atomistic Simulations." Zeolitic and Layered Material Gordon Research Conference. July 2005, Holyoke, MA. Poster & Invited short talk. Daniela Kohen.*
- "Carbon dioxide behavior in all silica zeolites." Third Midwest Undergraduate Computational Chemistry Symposium. July 2005, University of Minnesota. Talk. Jayme Dahlin,* Dorissa Zemirah* and Daniela Kohen.

- "Using atomistic simulations to study carbon dioxide diffusion in all silica zeolites." Third Midwest Undergraduate Computational Chemistry Symposium. July 2005, University of Minnesota. Talk. Disan Davis* and Daniela Kohen.
- "Do sodium cations help or hinder the adsorption of carbon dioxide on zeolites? – A progress report." Second Midwest Undergraduate Computational Chemistry Symposium. August 2004, University of Wisconsin, Madison. Talk. M. Thurlow* and Daniela Kohen.
- "Atomistic Simulation of Electrostatic Interactions: How to Treat Them when Simulating Carbon Dioxide and Other Gases in Zeolites." Second Midwest Undergraduate Computational Chemistry Symposium. August 2004, University of Wisconsin, Madison. Talk. Eric Feise* and Daniela Kohen.
- "Diffusion within zeolites – Atomistic simulations of Carbon Dioxide in Silica Zeolites." Second Midwest Undergraduate Computational Chemistry Symposium. August 2004, University of Wisconsin, Madison. Talk. Disan Davis* and Daniela Kohen.
- "Can a computational chemist help curb global warming?: Modeling the use of molecular sieves to isolate carbon dioxide." First Midwest Undergraduate Computational Chemistry Symposium. August 2003, Northwestern University. Talk. M. Thurlow,* Eric Feise,* Greg Haman* and Daniela Kohen.
- "Do sodium cations help or hinder the adsorption of carbon dioxide on zeolites?" First Midwest Undergraduate Computational Chemistry Symposium. August 2003, Northwestern University. Talk. M. Thurlow* and Daniela Kohen.
- "Modeling the adsorption of carbon monoxide on zeolites." First Midwest Undergraduate Computational Chemistry Symposium. August 2003, Northwestern University. Talk. Eric Feise* and Daniela Kohen.
- "Looking for carbon dioxide favorite spots within silicon and oxygen only zeolites." First Midwest Undergraduate Computational Chemistry Symposium. August 2003, Northwestern University. Talk. Greg Haman* and Daniela Kohen.
- "Mixing apples and oranges: a model study on non-adiabatic dynamics." First Midwest Undergraduate Computational Chemistry Symposium. August 2003, Northwestern University. Talk. D. Kohen,* J. C. Tully, and F. H. Stillinger.
- "Atomistic Simulations of CO_2 and N_2 Adsorption in Silica Zeolites: The Impact of Pore Size and Shape." American Conference in Theoretical Chemistry. July 2002, Champion, PA. Poster presentation. A.Goj, D. S. Sholl, E. D. Akten, and D. Kohen.*
- "Atomistic studies of the adsorption of CO_2/N_2 mixtures onto zeolites." ACS Undergraduate Poster Session, Orlando FL, 2002. A.Goj,* R.Siriwardane, D. S. Sholl, E. D. Akten, and D. Kohen.
- "Comparing Atomistic Simulations and Experimental Measurements of CO_2 selective Gas adsorption in zeolites." AIChE 2001 Annual Meeting. Talk. D. S. Sholl, R. Siriwardane, E. D. Akten, and D. Kohen.*

OTHER CONFERENCES ATTENDED

- LACOL (Liberal Arts Consortium for Online Learning) workshop. June 2014. Pomona College, CA.
- NOBCChE (National Organization for the Professional Advancement of Black Chemist and Chemical Engineers). Indiannapolis. October 2013. Organized and was a panelist in workshop " Your First Academic Position: Understanding Application Process, the Institutional Culture and the Expectations".
- John Gardner Institute Conference for Excellence in Gateway Course Completion. Indianapolis, IN. April, 2013
- SACNAS (Society for Advancement of Chicanos and Native Americans in Science). Seattle, WA. October 2012. Panelist in workshop "Academic Faculty Jobs at Primarily Undergraduate Institutions". Also chaperoned several FOCUS students.
- NOBCChE (National Organization for the Professional Advancement of Black Chemist and Chemical Engineers). Washington, DC. September 2012. Organized and was a panelist in workshop " Your First Academic Position: Understanding Application Process, the Institutional Culture and the Expectations".
- American Chemical Society National Meeting. San Diego, CA. March 2012.
- SACNAS (Society for Advancement of Chicanos and Native Americans in Science). San Jose, CA. October 2011. Chaperoned several FOCUS students.
- Institute on Teaching and Learning, Southern Regional Education Board (October, 2010):
- SACNAS (Society for Advancement of Chicanos and Native Americans in Science). Annaheim, CA. September 2010.
- NOBCChE (National Organization for the Professional Advancement of Black Chemist and Chemical Engineers). Atlanta, GA. March 2010.

- Student Migration Patterns In and Out of STEM Fields. April, 2008. Wingspread, WI.
- Symposia on Diversity on the Sciences IV. January, 2008. Chevy Chase, MA.
- 2nd annual Science of Diversifying Science Conference. June, 2007. UC Berkeley, CA.
- Symposia on Diversity on the Sciences II. October, 2006. Seattle, WA.
- American Chemical Society National Meeting. August 2005, Washington, DC.
- 8th International Conference on Fundamentals of Adsorption. May 2004, Sedona, AZ.
- American Chemical Society Great Lakes Regional Meeting. June 2002, Minneapolis, MN

OTHER INVITED TALKS:

- "Can a computational Chemist help curb global warming". Conversations on the wonder of science, a Northfield science café. Northfield, MN.
- "Being a Science Professor at a Predominantly Undergraduate Institution". Louisiana State University. April 2011

OTHER PROFESSIONAL ACTIVITIES:

- Member of the advisory board of the LS-PAC MODELS Center of Excellence. (Founded by NSF)
- Panelist in the Postdoc to Faculty workshop organized by the ACS. Denver, Co. August 2011. Indianapolis, IN. August 2013. San Francisco, CA. August 2014.
- Posse Mentor. 2011-13
- Organizer and co-founder of the Midwest Undergraduate Computational Chemistry Conference.
- Carleton's liaison to LACAFI (Liberal Arts College Association for Faculty Inclusion)
- Manuscript reviewer for Langmuir, the Journal of Physical Chemistry, the Journal of Chemical Physics, International Journal of Quantum Chemistry, Adsorption, and Industrial and Engineering Chemical Research.
- Proposal reviewer for NSF-career award, PRF and ResCorp.
- Participated in a MRI-NSF review panel. Arlington, Va. October 2009.
- Participated in a General Chemistry Discussion Forum, held by Pearson Publisher to discuss the new edition of their Introductory Chemistry textbook. Boston, MA. January 2010.

UNDERGRADUATE RESEARCH ADVISOR

- Anna Conley '20 (June 2018 - present)
- Elianna Frank '18 (June 2017 - June 2018). Graduate Student, Chemistry. University of California, Irvine.
- Brody Lynch '20 (January 2017 – January 2019)
- Will DeSnoo '19 (January 2017 – June 2019)
- Adam Nijhawan '19 (January 2017 – June 2019)
- Eliza Green (June 2014 – June 2015). Law Student, University of California, Berkeley.
- Katie Blise (March 2013 – June 2015). Graduate Student, Biomedical Engineering. Oregon Health and Sciences University. OR.
- Kit Pavlekovski (March 2013 – June 2014). Teaching for America. El Cerrito, CA.
- Nathan Bamberger (March 2013 – June 2015) Graduate Student, Chemistry, University of Arizona.
- Milan Cvitkovic (March 2012- June 2014). Graduate Student, Computing and Mathematical Sciences, Caltech.
- Annette Martin (March 2012-2013). Graduate student, Philosophy. New York University.
- Jie Lin (March 2012-2013). Master student, Applied Math and Theoretical Physics, Cambridge University.
- Diane Walters (March 2010- June 2012). Ph. D, Chemistry. University of Wisconsin, Madison. Process Engineer, Intel.
- Katie Deeg (June 2010- June 2012). Graduate student, Chemistry. University of California, Berkeley.
- Lindsey Madison (March 2008 – June 2010). Ph. D, Chemistry, Northwestern University. Assistant Professor, Colby College. ME.
- Henry Heitzer (March 2008 – June 2010). Ph. D. , Chemistry, Northwestern University. Boston Consulting

Group.

- Colin Russell (March 2008 – June 2010). Graduate student, Chemistry. University of Texas, Austin.
- Reed Jordan (March 2009 – June 2009). Master in City Planning Candidate, MIT
- David Selassie (March 2006 – June 2008). Master, Chemical Physics, Stanford University. Software Engineer at Simple.
- Felix Amankona-Diauwo (March 2006 – June 2008) Co-mentored by Mark Gordon at Iowa State University, IA. Ph. D., Chemistry, Northwestern University. Science Teacher at Latin High School, Chicago. IL
- Dorissah Zemirah (March 2005-June 2006). Medical school student, University of Minnesota.
- Jayme Dahlin (March 2004- August 2006) M. D. /Ph. D. student, Mayo Clinic.
- Disan Davis (March 2004- June 2006) Ph. D. Chemistry, Cornell University. Science Teacher at Hunter College High School.
- Meghan Thurlow (March 2003-June 2005). Ph.D. Chemistry, Harvard University. UCSF Postdoc.
- Eric Feise (March 2003- December 2005). Al engineer, Bungie, Communication Integration.
- Greg Haman (March 2003- March 2004). MD student, Harvard University.
- Anne Goj. (Smith College, 2001-2002) Ph. D. in Chemistry, Cornell University. Research Engineer at Transformer Protector.