

CURRICULUM VITAE

DANIELA KOHEN

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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. Associate Professor. General Chemistry, Chemical Thermodynamics, Statistical Thermodynamics, Advanced Kinetics Laboratory, Computational Chemistry, Time Dependent Quantum Mechanics, The Integrative Exercise. 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, Departamento 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, Departamento de Química Inorgánica, Analítica y Físico-Química. Undergraduate Research Assistant. Advisor: Miguel Blesa. 1988-1990.

ARTICLES

- “Atomistic Simulations of CO₂ and N₂ 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.
- “Atomistic Simulations of CO₂ and N₂ 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.
- “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.
- “Simulation of nonadiabatic wavepacket interferometry using classical trajectories.” *J. Chem. Phys.*, **112**, 7345 (2000). A. Donoso, D. Kohen and C. C. Martens.
- “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.
- “Phase space approach to dissipative molecular dynamics.” *Advances in Chemical Physics* **111**, 219 (2000). D. Kohen and D. J. Tannor.
- “Nanoscale shock wave spectroscopy: a direct view of coherent ultrafast bath dynamics.” *J. Phys. Chem.*, **111**, 4343 (1999). D. Kohen and C. C. Martens.
- “Model studies of non-adiabatic dynamics.” *J. Chem. Phys.*, **109**, 4713 (1998). D. Kohen, F. H. Stillinger and J. C. Tully.
- “Modeling the interactions of hydrogen with silicon surfaces.” *Surface Science*, **397**, 225 (1998). D. Kohen, J. C. Tully and F. H. Stillinger.
- “Classical-quantum correspondence in the Redfield equation and its solutions.” *J. Chem. Phys.*, **107**, 5141 (1997). D. Kohen and D. J. Tannor.
- “Phase space approach to theories of quantum dissipation.” *J. Chem. Phys.*, **107**, 5236 (1997). D. Kohen, C. C. Marston and D. J. Tannor.
- “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.
- “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.
- “Quantum adiabatic switching.” *J. Chem. Phys.* **98**, 3168 (1993). D. Kohen and D. J. Tannor.

RECENT AWARDS

- “Studying the behavior of CO₂ 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 Gustavus 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.

RECENT INVITED TALKS

- “ 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.

RECENT CONFERENCE PRESENTATIONS

- “Atomistic Simulations of CO₂ and N₂ in Silica Zeolites: The Impact of Pore Size and Shape” Foundations of Molecular Modeling and Simulations Conference. July 2009, Blaine, WA. Henry Heitzer*, Lindsey Madison*, Colin Russell*, and Daniela Kohen.
- “How do CO₂ and N₂ orient themselves within the ITQ-3 zeolite?” Mercury Conference on Computational Chemistry, Hamilton NY. July 2008. Lindsey Madison* and Daniela Kohen.
- “CO₂ and N₂ behavior within the LTA zeolite” Mercury Conference on Computational Chemistry, Hamilton NY. July 2008. Henry Heitzer* and Daniela Kohen.
- “Do Coulombic interactions dominate the rate of diffusion of CO₂ and N₂ within all-silica zeolites?” Mercury Conference on Computational Chemistry, Hamilton NY. July 2008. Colin Russell* and Daniela Kohen.
- “Atomistic Simulations of CO₂ and N₂ in Silica Zeolites: the impact of pore size and shape.” ACTC Conference, Northwestern University, Evanston, IL. July 2008. David Selassie*, Anne Goj, David S. Sholl, Jayme Dahlin*, Disan Davis* and Daniela Kohen.

- “Atomistic Simulations of CO₂ and N₂ 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 CO₂ and N₂ 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 CO₂ and N₂ Adsorption and Diffusion in Zeolites”. AIChE's Annual Meeting. November, 2007, Salt Lake City, UT
- “Carbon Dioxide and Nitrogen in Zeolites: Diffusion and Potential Energies” Sixth Midwest Undergraduate Computational Chemistry Symposium. August 2007, Champaign-Urbana, IL. Talk. David Selassie * and Daniela Kohen
- “Using the Effective Fragment Potential in atomistic simulation of CO₂ adsorption in Zeolites” Sixth Midwest Undergraduate Computational Chemistry Symposium. August 2007, Champaign-Urbana, IL. 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, Ames, IA. Talk. Felix Amankona-Diawuo,* David Selassie* and Daniela Kohen.
- “Analysis of the preferred Sites of CO₂ and N₂ in silica zeolites.” Fourth Midwest Undergraduate Computational Chemistry Symposium. August 2006, Ames, IA. Talk. Jayme Dahlin* and Daniela Kohen.
- “Studying CO₂ 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 CO₂ 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, Minneapolis, MN. 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, Minneapolis, MN. 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, Madison, WI. 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, Madison, WI. 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, Madison, WI. 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, Evanston, IL. 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, Evanston, IL. Talk. M. Thurlow* and Daniela Kohen.

➤ "Modeling the adsorption of carbon monoxide on zeolites." First Midwest Undergraduate Computational Chemistry Symposium. August 2003, Evanston, IL. 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, Chicago, IL. 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, Chicago, IL. Talk. D. Kohen,* J. C. Tully, and F. H. Stillinger.

➤ "Atomistic Simulations of CO₂ and N₂ 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 CO₂/N₂ 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 CO₂ selective Gas adsorption in zeolites." AIChE 2001 Annual Meeting. Talk. D. S. Sholl, R. Siriwardane, E. D. Akten, and D. Kohen.*

OTHER CONFERENCES ATTENDED

- 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 PROFESSIONAL ACTIVITIES:

- Organizer and co-founder of the Midwest Undergraduate Computational Chemistry Conference.
- Manuscript review for *Langmuir*, the *Journal of Physical Chemistry*, *International Journal of Quantum Chemistry*, *Adsorption*, and *Industrial and Engineering Chemical Research*.
- Proposal review for NSF-career award and PRF.