David W.H. Swenson

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Education

2005-2011 **University of California, Berkeley**, *Doctor of Philosophy*
Field: Physical Chemistry, Advisor: William H. Miller
Dissertation: "Quantum Effects from Classical Trajectories: New Methods and Applications for Semiclassical Dynamics."

2003-2005 **Université Louis Pasteur**, *Diplôme d'Études Universitaires Générales*
Field: Mathématiques, Informatique, et Applications aux Sciences
Undergraduate degree in "mathematics, computer science, and applications to the sciences."

1999-2003 **Colorado College**, *Bachelor of Arts*
Majors: Chemistry, French Literature, and Physics

1998-1999 **Indiana University-Purdue University, Indianapolis**
Upper-division classes in French taken concurrently with senior year in high school.

Awards

1999-2003 **Otis A. and Margaret T. Barnes Scholarship**, *Colorado College*
A four-year, full-tuition scholarship for chemistry majors.

1999-2003 **Central Newspapers Foundation Scholarship**, *Central Newspapers Foundation*
A four-year, $10,000 scholarship for children of employees of Central Newspapers, Inc.

Research Employment Experience

2012 – Present **Universiteit van Amsterdam**, *Post-Doctoral Fellow*
Field: Theoretical Chemistry (Rare Events), Advisor: Peter G. Bolhuis
- Developed multiple interface set transition interface sampling to study networks of rare events.
- Co-principal developer of OpenPathSampling, a software package to study rare events.
- Developed a mathematical framework (path ensemble theory) underlying OpenPathSampling.
- Planned and guided undergraduate research projects. Assisted graduate students with research.
- Formed collaborations with other researchers to study systems of biological importance.

Sep 2015 – Dec 2015 **Memorial Sloan Kettering Cancer Center**, *Visiting Post-Doctoral Fellow*
Field: Computational Biology, Advisor: John D. Chodera
- Continued development of OpenPathSampling.

Aug 2011 – Dec 2011 **Tel Aviv University**, *Visiting Post-Doctoral Fellow*
Field: Theoretical Chemistry (Molecular Electronics), Advisor: Eran Rabani
- Extended my "dynamics for classically mapped fermions" approach to more complicated systems.

2005–2011 **University of California, Berkeley**, *Graduate Student Researcher*
Field: Theoretical Chemistry (Semiclassical Dynamics), Advisor: William H. Miller
- Developed new methods for calculating the semiclassical prefactor.
- Developed methods to reduce the number of trajectories for semiclassical calculations.
- Created "dynamics for classically mapped fermions," a semiclassical method for fermion dynamics.
- Applied my "dynamics for classical mapped fermions" method to models of molecular conduction.

Sept 2008 – Jan 2009 **D. E. Shaw Research, LLC**, *Research Intern*
Field: Theoretical Chemistry/Computational Biology, Manager: John Klepeis
- Beta-tested a new parallel framework for trajectory analysis, based on the map-reduce approach used by Google.
- Verified selfdiffusion, viscosity, and orientational correlation of a novel water model.

Summers 2003-2005 **Indiana University-Purdue University Indianapolis**, *Summer Researcher*
Field: Theoretical Chemistry, Advisor: Clifford E. Dykstra
- Developed a potential energy surface to describe molecular hydrogen clustering around benzene.
- Applied my model to study clusters of up to 20 hydrogen molecules around a single benzene.

Summer 2002 **Université Bordeaux I**, *REU Exchange Student*
Field: Theoretical Chemistry, Advisors: Jean-Claude Rayez and Laurent Bonnet
- Began work on a quasiclassical trajectory simulation to determine product state distributions from the associative desorption of hydrogen from a Pt(1 1 1) surface.

Summer 2001 **University of Oregon**, *REU Student*
Field: Theoretical Chemistry, Advisor: Jeffrey A. Cina
- Studied the potential energy surface of the I_2–Ar system in preparation for theoretical studies of the pump-probe spectroscopy of I_2 in an argon matrix.
- Explored the viability of using a computer algebra system as a tool in theoretical chemistry.

Summer 2000 **Colorado College**, *Summer Researcher*
Field: Natural Product Synthesis, Advisors: Nick Drapela and Ted Lindeman
- Steps toward the synthesis of candidate anti-tumor agent sequoiatone A.

Service and Volunteer Activities

2013-2015 **Group Outing Organization Committee**, *Molecular Simulation Group*
Helped plan activities for a group outing that had scientific value and was also fun for the participants. Designed several games based on useful scientific skills such as reading and presenting scientific literature, and explaining scientific concepts. Organized some logistical aspects of the outing.

2002-2003 **Student Representative to Department Meetings**, *Colorado College*
Elected by fellow students to represent their interests at Chemistry Department meetings. Organized student involvement in the hiring of a new professor.

2000-2003 **Kids' Science Day**, *Colorado College*
Program to introduce elementary school students to fun parts of science. Helped organize the first annual event, and served as counselor or chemistry/physics demonstrator every year.

1999-2003 **Student Affiliates of the American Chemical Society**, *Colorado College*
Served in several roles, including editor of the department newsletter, outreach coordinator, co-coordinator of National Chemistry Week activities, and executive vice president.

Teaching Experience

Apr-Jun 2014 **Bachelor's Thesis Project**, *Universiteit van Amsterdam (Supervisor)*
Proposed, supervised, and helped design a research project to serve as the thesis project for a Bachelor's student.

Jun 2013 **Second-Year Student Project**, *Universiteit van Amsterdam (Supervisor)*
Designed, planned, and supervised a one-month research project for second-year undergraduates studying chemistry. Results from this project were presented in one of my talks at the 246th ACS National Meeting.

Every January 2013–2015 **Molecular Simulation Tutorial**, *Universiteit van Amsterdam (Teaching Assistant)*
Course for graduate students and post-docs in the field of computational chemistry. Guided several computer lab sessions.

Fall 2010 **General Chemistry**, *University of California, Berkeley (Teaching Assistant)*
Instructors: John Arnold, Angela Stacy, Marcin Majda, and Michelle Douskey

Fall 2007 **Advanced Quantum Mechanics**, *University of California, Berkeley (Teaching Assistant)*
Instructor: Daniel M. Neumark
Sole teaching assistant for a graduate-level course taken by most physical chemistry graduate students.

Fall 2006 **Physical Chemistry**, *University of California, Berkeley (Teaching Assistant)*
Instructors: William H. Miller and Haw Yang
Undergraduate course to introduce chemistry majors to quantum mechanics.

Fall 2005 **General Chemistry**, *University of California, Berkeley (Teaching Assistant)*
Instructors: Richard Saykally, Mark Kubinec, and Michelle Douskey
Introduction to chemical principles for non-majors.

2003-2004 **English Assistant**, *Lycée Le Corbusier (Illkirch, France)*
Taught English (as a foreign language) in a French high school focused on construction-related employment. My students ranged from housepainter apprentices to those who planned to become architects and designers.

1999-2003 **Chemistry and Physics Tutor**, *Colorado College*
Helped students in lower division chemistry and physics classes with homework and lab reports.

Miscellaneous

Languages *English*: native.
French: proficient (CEFR B2+).
Dutch: intermediate (CEFR B1/B2).

Programming *Preferred programming languages*: Python, C, C++.
Experienced with: Fortran 77, Perl, bash, awk, Mathematica.
Some experience with: PHP, CaML, Maple, Matlab/Octave, R, Fortran 90, Pascal.

Other Amateur radio Extra class license (highest level possible; station: K9ECP).
Other hobbies: photography, harp, distance bicycling, mountain climbing, and travel.

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Publications and Presentations

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Publications

David W.H. Swenson and Peter G. Bolhuis. "A replica exchange transition interface sampling method with multiple interface sets for investigating networks of rare events." *J. Chem. Phys.* **141**, 044101 (2014).

Bin Li, Tal J. Levy, David W.H. Swenson, Eran Rabani, and William H. Miller. "A Cartesian Quasi-classical Model to Nonequilibrium Quantum Transport: The Anderson Impurity Model." *J. Chem. Phys.* **138**, 104110 (2013).

David W.H. Swenson, Guy Cohen, and Eran Rabani. "A semiclassical model for the non-equilibrium quantum transport of a many-electron Hamiltonian coupled to phonons." *Mol. Phys.* **110**, 743 (2012).

David W.H. Swenson, Tal Levy, Guy Cohen, Eran Rabani, and William H. Miller. "Application of a semiclassical model for the second-quantized many-electron Hamiltonian to nonequilibrium quantum transport: The resonant level model." *J. Chem. Phys.* **134**, 164103 (2011).

David W.H. Swenson, Heather M. Jaeger, and Clifford E. Dykstra. "Clustering of molecular hydrogen around benzene." *Chem. Phys.* **326**, 329 (2006).

Heather M. Jaeger, David W.H. Swenson, and Clifford E. Dykstra. "Feature Article: Remarkable Features in the Interactions of Quadrupolar Molecules." *J. Phys. Chem. A* **110**, 6399 (2006).

Publications in preparation

David W.H. Swenson, Martin Spruijt, Imke van Rees, and Peter G. Bolhuis. "Studying 'rarer' transitions using multiple interface set transition interface sampling." (Preliminary results shown in oral presentation at 246th ACS National Meeting).

Jan-Hendrik Prinz, David W.H. Swenson, Peter G. Bolhuis, and John D. Chodera. "OpenPathSampling: A flexible, open framework for path sampling simulations. I. Basics." (Presented at Dutch Molecular Dynamics Day, February 27, 2015).

David W.H. Swenson, Jan-Hendrik Prinz, John Chodera, and Peter G. Bolhuis. "OpenPathSampling: A flexible, open framework for path sampling simulations. II. Advanced Topics." (Presented at Dutch Molecular Dynamics Day, February 27, 2015).

David W.H. Swenson, Jan-Hendrik Prinz, John Chodera, and Peter G. Bolhuis. "Path Ensemble Theory: A general mathematical treatment of path sampling."

Jocelyne Vreede and David W.H. Swenson. "Mechanism and rates for the Watson-Crick to Hoogsteen 'base rolling' transition in B-DNA." (Preliminary results shown on poster at 246th ACS National Meeting).

Eva van Mastbergen, David W.H. Swenson, and Jocelyne Vreede. "Avoiding problems in short-oligomer simulations of DNA-protein binding."

David W.H. Swenson. "Bingo sampling: An efficient approach to time-dependent importance sampling, with applications to semiclassical time correlation functions." (Preliminary results can be seen at `http://vimeo.com/76616662`).

David W.H. Swenson. "Important initial phase space distribution in semiclassical calculations as a predictor of quantum interference effects." (Preliminary results shown in oral presentation at 246th ACS National Meeting).

Oral Presentations

David W.H. Swenson. "OpenPathSampling: An open, flexible Python framework for rare event simulations." Duch Molecular Dynamics Day 2015: Amsterdam, Netherlands. February 27, 2015.

David W.H. Swenson and Peter G. Bolhuis. "Numerical study of correlated rare events using replica exchange multiple state transition interface sampling." Eleventh International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computating.: Leuven, Belgium. April 6-11, 2014.

David W.H. Swenson. "Sampling networks of rare events with multiple interface set transition interface sampling." Dutch Molecular Dynamics Day 2014: Enschede, Netherlands. March 7, 2014.

David W.H. Swenson and Peter G. Bolhuis. "Numerical study of correlated rare events using replica exchange multiple state transition interface sampling." 246th American Chemical Society National Meeting: Indianapolis, Indiana. September 8, 2013.

David W.H. Swenson. "Important initial phase space distributions in semiclassical dynamics and the nature of quantum coherences." 246th American Chemical Society National Meeting: Indianapolis, Indiana. September 8, 2013.

David W.H. Swenson. "A Classical Model for Nonequilibrium Quantum Transport: The Dynamics for Classically Mapped Fermions Method." Amsterdam Center for Multiscale Modeling Symposium: Amsterdam, The Netherlands. June 28, 2012.

David W.H. Swenson. "Classical Dynamics for Nonequilibrium Quantum Transport: The Dynamics for Classically Mapped Fermions Method." Dutch Molecular Dynamics Day: Groningen, The Netherlands. March 23, 2012.

David W.H. Swenson, Tal Levy, Guy Cohen, Eran Rabani, and William H. Miller. "Semiclassical model for fermion dynamics (with applications to molecular electronics)." 242nd American Chemistry Society National Meeting: Denver, Colorado. August 28, 2011.

Poster Presentations

David W.H. Swenson. "Efficient sampling of large rare event networks with multiple state replica exchange transition interface sampling." CECAM Workshop: Long time dynamics from short time simulations: Lugano, Switzerland. March 12-14, 2014.

David W.H. Swenson. "Beyond basic molecular dynamics: New tools for the study of molecules in motion." 246th American Chemical Society National Meeting: Indianapolis, Indiana. September 9, 2013.

David W.H. Swenson. "Transition Path Sampling Applied to Semiclassical IVRs." Mini Statistical Mechanics Meeting: Berkeley, California. January 14-16, 2011.

David W.H. Swenson and William H. Miller. "Monodromy matrix calculation by the precision finite difference method." 239th American Chemical Society National Meeting: San Francisco, California. March 21-25, 2010.

David W.H. Swenson and Cristian Predescu. "A Method for Solving Poisson Problems." Mini Statistical Mechanics Meeting: Berkeley, California. January 12-14, 2007.

David W.H. Swenson, Laurent Bonnet, and Jean-Claude Rayez. "The State Distribution of the Associative Desorption of H_2 from a Pt(1 1 1) Surface." 2002 Undergraduate Research Poster Session: Gainesville, Florida. October 25-27, 2002.

David W.H. Swenson and Jeffrey A. Cina. "Exploring the Ground State Potential of I_2-Ar." Inter-REU Workshop: 1st US/France Chemistry and Communication Meeting: Strasbourg, France. June 13-15, 2002.