David W.H. Swenson

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Education

2005 – 2011 **University of California, Berkeley**, *Doctor of Philosophy*
Field: 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.

Research Employment Experience

2018 – **École Normal Supérieure de Lyon**, *Post-Doctoral Researcher*
Theoretical Chemistry, Advisor: Ralf Everaers

2012 – 2018 **Universiteit van Amsterdam**, *Post-Doctoral Fellow*
Theoretical Chemistry (Rare Events), Advisor: Peter G. Bolhuis

2015 **Memorial Sloan Kettering Cancer Center**, *Visiting Post-Doctoral Fellow*
Computational Biology, Advisor: John D. Chodera

2011 **Tel Aviv University**, *Visiting Post-Doctoral Fellow*
Theoretical Chemistry (Molecular Electronics), Advisor: Eran Rabani

2005 – 2011 **University of California, Berkeley**, *Graduate Student Researcher*
Theoretical Chemistry (Semiclassical Dynamics), Advisor: William H. Miller

2008 – 2009 **D. E. Shaw Research, LLC**, *Research Intern*
Theoretical Chemistry/Computational Biology, Manager: John Klepeis

Summers **Indiana University-Purdue University Indianapolis**, *Summer Researcher*
2003 – 2005 Theoretical Chemistry, Advisor: Clifford E. Dykstra

Summer 2002 **Université Bordeaux I**, *REU Exchange Student*
Theoretical Chemistry, Advisors: Jean-Claude Rayez and Laurent Bonnet

Summer 2001 **University of Oregon**, *REU Student*
Theoretical Chemistry, Advisor: Jeffrey A. Cina

Summer 2000 **Colorado College**, *Summer Researcher*
Natural Product Synthesis, Advisors: Nick Drapela and Ted Lindeman

Teaching Experience

2016 –2018 **Master's Thesis Project**, *Universiteit van Amsterdam (Supervisor)*
Daily supervisor for the thesis project of a master's student.

Apr–Jul 2018 **Bachelor's Thesis Project**, *Universiteit van Amsterdam (Supervisor)*

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, 2017 **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.

Conference Organization

2019 **ESDW: Topics in Classical MD**, *(Organizer)*
Lyon, France

2018 **Extended Software Development Workshop: Intelligent high throughput computing for scientific applications**, *(Organizer)*
Turin, Italy

2017 **E-CAM Extended Software Development Workshop: Classical MD**, *(Organizer)*
Leiden, Netherlands

2017 **Dutch Molecular Dynamics Day 2017**, *(Session Chair)*
Delft, Netherlands

2016 **E-CAM Extended Software Development Workshop: Path Sampling**, *(Organizer)*
Traunkirchen, Austria

Service and Volunteer Activities

2015–Present **E-CAM Work Package 1 Co-Leader**

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.

Funded Proposals

2019 **ESDW: Topics in Classical MD**, *Principal proposal author*
Funding agency: CECAM. Award amount: 21000

2018 **Extended Software Development Workshop: Intelligent high throughput computing for scientific applications**, *Principal proposal author*
Funding agency: CECAM. Award amount: 23000

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.

Publications

2019 David W.H. Swenson, Jan-Hendrik Prinz, Frank Noé, John D. Chodera, and Peter G. Bolhuis. "OpenPathSampling: A flexible, open framework for path sampling simulations. 1. Basics." *J. Chem. Theory Comput.* **15**, 813 (2019).

2019 David W.H. Swenson, Jan-Hendrik Prinz, Frank Noé, John D. Chodera, and Peter G. Bolhuis. "OpenPathSampling: A flexible, open framework for path sampling simulations. 2. Building and Customizing Path Ensembles and Sample Schemes." *J. Chem. Theory Comput.* **15**, 837 (2019).

2017 Arthur C. Newton, Ramses Kools, David W.H. Swenson, and Peter G. Bolhuis. "The two opposing effects of isotropic and anisotropic attraction on the association kinetics of patchy particles." *J. Chem. Phys.* **147**, 115101 (2017).

2014 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).

2013 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).

2012 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).

2011 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).

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

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

Submitted Jocelyne Vreede, Peter G. Bolhuis, and David W.H. Swenson. "Atomistic insight into the kinetic pathways for Watson-Crick to Hoogsteen transitions in DNA." (Submitted).

Sander Roet, Ferry Hooft, Peter G. Bolhuis, David W.H. Swenson, and Jocelyne Vreede. "Path sampling simulations show the effect of the Q61L mutation in the dynamics of K-Ras."

Invited Talks

2018 David W.H. Swenson. "Path sampling of medically relevant biomolecular systems: Old and new tricks with OpenPathSampling." E-CAM State-of-the-Art Workshop: Large scale activated event simulations: Vienna, Austria. October 1–3, 2018.

2018 David W.H. Swenson. "Task-based parallelization of replica exchange transition interface sampling in OpenPathSampling." Platform for Advanced Scientific Computing Conference (PASC18): Basel, Switzerland. July 2–4, 2018.

2018 David W.H. Swenson. "Path sampling and the LAMMPS interface for OpenPathSampling." LAMMPS for molecular dynamics simulations: from development to applications: Lyon, France. June 26, 2018.

2018 David W.H. Swenson. "Using path sampling for atomistic insight into the kinetics and dynamics of medically relevant biomolecules." Building the bridge between theories and software: SME as a boost for technology transfer in industrial simulative pipelines: Genoa, Italy. May 23–25, 2018.

2017 David W.H. Swenson. "OpenPathSampling: A Python package for investigating biomolecular rare event simulations." Automation in Biomolecular Simulation and Modeling: Amsterdam, Netherlands. September 12, 2017.

2016 Jocelyne Vreede, Peter G. Bolhuis, David W.H. Swenson. "Simulating the mechanisms and rates of transitions between Watson-Crick and Hoogsteen base pairing." NWO CHAINS 2016: Veldhoven, Netherlands. December 8, 2016.

2016 David W.H. Swenson. "Introduction to OpenPathSampling: Overview and Usage." CECAM Extended Software Development Workshop: Trajectory Sampling: Traunkirchen, Austria. November 17, 2016.

2015 David W.H. Swenson. "Quantum dynamics from classical trajectory simulations." Brown University: Providence, Rhode Island. December 8, 2015.

2014 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 Computing.: Leuven, Belgium. April 6-11, 2014.

2012 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.

Contributed Talks

2017 David W.H. Swenson. "Scalability of Path Sampling Simulations." E-CAM Extreme-Scale State of the Art Workshop: Barcelona, Spain. July 6, 2017.

2016 David W.H. Swenson, Jan-Hendrik Prinz, John D. Chodera, Peter G. Bolhuis. "Generation and Analysis of Arbitrary Path Ensembles using OpenPathSampling." CECAM Workshop: Reaction Coordinates from Molecular Trajectories: Leiden, Netherlands. September 1, 2016.

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

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.

2013 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.

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.

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.

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

Guest Lectures / Teaching Talks

2016 David W.H. Swenson. "Tutorial: Software testing in scientific programming." CECAM Extended Software Development Workshop: Trajectory Sampling: Traunkirchen, Austria. November 21, 2016.

Poster Presentations

2018 David W.H. Swenson. "Path sampling: Software and practical applications." CECAM/CSM/IRTG School 2018: Machine Learning in Scientific Computing: Nierstein, Germany. September 10–14, 2018.

2017 David W.H. Swenson. "OpenPathSampling: A flexible Python framework for rare events." Recent Advances in Modeling Rare Events (RARE 2017): Agra, India. December 7-10, 2017.

2017 David W.H. Swenson. "Path sampling for unbinding kinetics." 3rd E-CAM General Assembly: Barcelona, Spain. November 29-30, 2017.

2014 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.

2013 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.

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

2010 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.

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

2002 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.

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.

Miscellaneous

Languages
English: native
French: proficient
Dutch: advanced

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).