David W.H. Swenson

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Overview

- Employed in **computational molecular science** since a summer 2001 undergraduate project.
- Experience includes **software development**, **method development**, and **applications to scientific problems** of interest, ranging from simple models to all-atom biomolecular simulations.
- Areas of contributions include **force field development**, **quantum dynamics**, **enhanced sampling** of rare events, and **alchemical free energy calculations**.

Employment Experience

2022 – **Open Molecular Software Foundation**, *Senior Software Scientist*
Infrastructure Lead, Open Free Energy
- Contributed to open-source software for alchemical free energy calculations.
- Led work to emphasize developer experience and user experience in software design.

2018 – 2021 **École Normale Supérieure de Lyon**, *Post-Doctoral Researcher*
Computational Chemical Physics, Advisor: Ralf Everaers
- Continued development of OpenPathSampling.
- Ensured that progress was made on grant deliverables and wrote annual deliverable reports.

2012 – 2018 **Universiteit van Amsterdam**, *Post-Doctoral Fellow*
Theoretical Chemistry (Rare Events), Advisor: Peter G. Bolhuis
- Developed new path sampling methods to study networks of rare events.
- Co-principal developer of OpenPathSampling, a software package to study rare events.
- Planned and supervised undergraduate and master's research projects.
- Formed collaborations with other researchers to study systems of biological importance.

Visiting Positions

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

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

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

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.

Open Source Software Experience

Preferred programming languages: Python, C, C++, bash
Comfortable with many other languages.

Maintainer of **12 projects on PyPI** and **13 projects on conda-forge**. Contributed pull requests into **dozens of GitHub repositories** owned by **over 20 users and organizations**.

Some contribution highlights include:

Major contributor

OpenPathSampling: `https://github.com/openpathsampling/openpathsampling`
Python library for path sampling; ∼45000 lines of code.

OpenFE: `https://github.com/openfreeenergy/openfe`
Python toolkit for free energy calculations; ∼20000 lines of code.

Contact Map Explorer: `https://github.com/dwhswenson/contact_map`
Python tool for contact maps; ∼3500 lines of code.

Contributor (selected)

MDTraj: `https://github.com/mdtraj/mdtraj`

OpenMMTools: `https://github.com/choderalab/openmmtools`

betterbib: `https://github.com/texworld/betterbib`

UltraJSON: `https://github.com/ultrajson/ultrajson`

For more, see my profile at **`https://github.com/dwhswenson`**.

Academic Activities

Publications

- **13 peer-reviewed publications** (h-index 10)
- 6 first author; 1 last/sole corresponding author
- Recently receiving approximately **200 citations per year**
- Details on Google Scholar (includes some work that was not peer-reviewed): `https://tinyurl.com/DWHSwensonScholar`

Presentations

Frequent speaker at national and international meetings on chemistry and computational science. Recent highlights:

- Contributed talk at **US Research Software Engineers Association** (Chicago, 2023)
- Invited talk at **University of Amsterdam** (2022)
- Invited talk at workshop **"Electronic Structure Software Development: Best Practices and Tools"** (Lausanne, 2022)
- Contributed talk at **ACS Fall 2022** (Chicago)
- Contributed talk at **APS March Meeting 2021** (Virtual)

Conference Organization

Organized **4 European conferences** on scientific software development:

- 2 on task-based parallel computing, 2 on developing software for molecular dynamics
- **Wrote funding proposal** for 2, obtaining €21000 for one and €23000 for the other

Teaching

- Guest Lecturer for a Master's course in **Biomolecular Simulation** at the University of Amsterdam in 4 different years.
- Prepared and gave tutorial on **Software Testing for Scientific Programming** at 4 different E-CAM Extended Software Development Workshops.
- Teaching assistant for **graduate-level quantum mechanics**, undergraduate **physical chemistry**, and **general chemistry** at University of California, Berkeley.
- Taught **English** at a French high school for an academic year (2003-2004).

Supervision

1 Master's thesis, 1 Master's internship, 2 Bachelor's theses