

Stéphanie Valleau, Ph.D.

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Academic appointments

University of Washington <i>Assistant Professor</i>	Seattle, WA 2019–Present
University of Washington <i>Affiliate Faculty - eScience Institute</i>	Seattle, WA 2020–Present

Education

Stanford University <i>Simons Foundation Postdoctoral Research Fellow</i> Simons Collaboration on the Origins of Life (SCOL) SCOL Project: Atomistic exploration of abiogenesis with a nanoreactor.	Stanford, CA 2016–2019
Harvard University <i>PhD in Physical Chemistry with Secondary Field in Computer Science</i> Dissertation title: Theoretical study of exciton transport in natural and synthetic light-harvesting systems.	Cambridge, MA 2010–2016
Harvard University <i>Master's of Arts (AM) in Physics</i>	Cambridge, MA 2013
Università degli Studi di Milano <i>Master's of Science in Physical Chemistry</i> Honors degree with grade 110/110 <i>Cum Laude</i> Thesis title: A Quantum Instanton study of the diffusion of hydrogen and its isotopes on Ni(100).	Milan, Italy 2008–2010
Università degli Studi di Milano <i>Bachelor's of Science in Chemistry</i> Honors Degree with grade 110/100 <i>Cum Laude</i> Thesis title: Quantum dynamics of the diffusion of hydrogen and its isotopes on Ni(100).	Milan, Italy 2005–2008

Awards & Fellowships

Simons Collaboration on the Origins of Life postdoctoral fellowship <i>Simons Foundation postdoctoral fellowship</i> World-wide competition for a three-year postdoctoral fellowship from the Simons Collaboration on the Origins of Life.	Stanford University 2016
ACS award in Computational Physical Chemistry <i>Graduate student award</i> Nation-wide competition among graduate students in theoretical and computational chemistry, award includes 100K hours of computational time on the Blue Waters supercomputer.	Harvard University 2013
Martin Karplus award <i>Graduate student award</i>	Harvard University 2010

Conference Presentations

S. Valleau, *Invited Talk*: Machine learning quantum reaction rate constants, CBE Computing Seminar Series University of Wisconsin-Madison, Virtual, February 2021.

S. Valleau, *Invited Talk*: Machine learning reactivity in networks of coupled gas phase reactions, AIChE Annual Meeting, Virtual, November 2020.

S. Valleau, *Talk*: Machine learning quantum tunneling in the kinetics of chemical reactions, AIChE Annual Meeting, Virtual, November 2020.

N. Janulaitis and **S. Valleau**, *Poster*: Computational Study of Ground State Organic Chemistry Reactions in the Presence of Toxic and Non-Toxic Solvents, AIChE Annual Meeting, Virtual, November 2020.

E. Komp and **S. Valleau**, *Poster*: Towards predicting kinetics in systems of coupled reactions with deep neural networks, AIChE Annual Meeting, Virtual, November 2020.

S. Valleau, *Lightning Talk*: Machine learning quantum reaction rate constants, Conference on Theoretical Chemistry, Virtual, June 2020.

N. Janulaitis and **S. Valleau**, *Poster*: A computational study of the kinetics of the menshutkin reaction, Conference on Theoretical Chemistry, Virtual, June 2020.

E. Komp and **S. Valleau**, *Poster*: Predicting quantum rate constants in one dimension with machine learning, Conference on Theoretical Chemistry, Virtual, June 2020.

S. Valleau, *Poster*: Reaction dynamics of cyanohydrines with hydrosulfide in water, Molkin Conference, Berlin, June 2019.

S. Valleau, *Poster*: Ab-Initio molecular dynamics simulation of prebiotic RNA replication, SCOL Annual symposium, New York, April 2019.

S. Valleau, *Poster*: Theoretical study of cyanohydrin reactions with hydrogen sulfide in the context of origins of life, Computational Chemistry Gordon Research Conference, Mount Snow, VT, July 2018.

S. Valleau, *Poster*: Theoretical study of cyanohydrin reactions with hydrogen sulfide in the context of origins of life, Computational Chemistry Gordon Research Conference, Mount Snow, VT, July 2018.

S. Valleau, *Poster*: Reaction dynamics of cyanohydrins with hydrosulfide in water, SCOL Annual symposium, New York, April 2018.

S. Valleau, *Poster*: Reaction dynamics of cyanohydrins with hydrogen sulfide in the context of origins of life, WCTC conference, Stanford, March 2018.

S. Valleau, *Talk*: Exploration of abiogenesis with a nanoreactor, SCOL Investigators and Fellows Meeting, New York, November 2017.

S. Valleau, *Poster*: Dynamics of reactions fundamental to the origins of life, ACTC conference, Boston, July 2017.

S. Valleau, *Invited talk*: Evolution of the Fenna-Matthews-Olson complex, PBI conference, Harvard, May 2016.

S. Valleau, *Poster*: Evolution of the Fenna-Matthews-Olson complex, CIFAR meeting, San Francisco, December 2015.

S. Valleau, S. Saikin, D. Ansari, M. Rostami, H. Mosallaei, A. Aspuru-Guzik, *Poster*: Electromagnetic study of the chlorosome antenna complex of *Chlorobaculum tepidum*, QuEBS2015, Florence, July 2015.

S. Valleau, S. Saikin, D. Ansari, M. Rostami, H. Mosallaei, A. Aspuru-Guzik, *Contributed Talk*: Electromagnetic study of the chlorosome antenna complex of *Chlorobaculum tepidum*, QUITEL2014, San Cristobal, November 2014.

S. Valleau, S. Saikin, D. Ansari, M. Rostami, H. Mosallaei, A. Aspuru-Guzik, *Contributed Talk*: Electromagnetic study of the chlorosome antenna complex of *Chlorobaculum tepidum*, CCP2014, Boston, August 2014.

S. Valleau, *Talk*: Exciton transport in J-aggregates of cyanine dyes and hybrid J-aggregate - photonic structures, OQS center, Cambridge, April 2012.

S. Valleau, S. Saikin, M. Yung and A. Aspuru-Guzik, *Contributed Talk*: Study of excitonic energy transport in thin-film J-aggregates, APS-March meeting, Boston, March 2012.

S. Valleau, S. Saikin, M. Yung and A. Aspuru-Guzik, *Poster*: Exciton dynamics in thin film J-aggregates, CECAM Conference, Bremen, June 2011.

Publications

- [1] E. Komp and **S. Valleau**. Machine learning quantum reaction rate constants. *J. Phys. Chem. A.*, 124(41):8607–8613, 2020.
- [2] **S. Valleau** and T. J. Martínez. Reaction dynamics of cyanohydrins with hydrosulfide in water. *J. Phys. Chem. A.*, 123:7210–7217, 2019.
- [3] **S. Valleau**, R. A. Studer, F. Häse, C. Kreisbeck, R. G. Saer, R. E. Blankenship, E. I. Shakhnovich, and A. Aspuru-Guzik. Absence of selection for quantum coherence in the fenna-matthews-olson complex: A combined evolutionary and excitonic study. *ACS Central Science*, 3(10):1086–1095, 2017.
- [4] F. Häse, **S. Valleau**, E. Pyzer-Knapp, and A. Aspuru-Guzik. Machine learning exciton dynamics. *Chem. Sci.*, 7:5139, 2016.
- [5] S. Chandrasekaran, M. Aghtar, **S. Valleau**, A. Aspuru-Guzik, and U. Kleinekathoefer. Influence of force fields and quantum chemistry approach on spectral densities of bchl a in solution and in fmo protein. *J. Phys. Chem. B.*, 119:9995, 2015.
- [6] **S. Valleau**, S. Saikin, D. Ansari-Oghol-Beig, M. Rostami, H. Mosallaei, and A. Aspuru-Guzik. Electrodynamic study of the chlorosome antenna complex in chlorobium-tepidum. *ACS Nano*, 8:3884, 2014.
- [7] J. Huh, S. Saikin, J. Brookes, **S. Valleau**, T. Fujita, and A. Aspuru-Guzik. Atomistic study of energy funneling in the light-harvesting complex of green sulfur bacteria. *JACS*, 136:2048–2057, 2014.
- [8] D. Ansari-Oghol-Beig, M. Rostami, E. Chernobrovkina, S. Saikin, **S. Valleau**, H. Mosallaei, and A. Aspuru-Guzik. Parametric hierarchical matrix approach for the wideband optical response of large-scale molecular aggregates. *J. App. Phys.*, 114:164315, 2013.
- [9] S. Mandrà, **S. Valleau**, and M. Ceotto. Deep nuclear resonant tunneling thermal rate constant calculations. *Int. J. Quant. Chem.*, 113:1722, 2013.
- [10] S. Saikin, A. Eisfeld, **S. Valleau**, and A. Aspuru-Guzik. Photonics meets excitonics: natural and artificial molecular aggregates. *Nanophotonics*, 2:21, 2013.
- [11] **S. Valleau**, A. Eisfeld, and A. Aspuru-Guzik. On the alternatives for bath correlators and spectral densities from mixed quantum-classical simulations. *J. Chem. Phys.*, 137:224103, 2012.
- [12] **S. Valleau**, S. K. Saikin, M-H. Yung, and A. Aspuru-Guzik. Exciton transport in thin-film cyanine dye j-aggregates. *J. Chem. Phys.*, 137:034109, 2012.
- [13] S. Shim, P. Rebentrost, **S. Valleau**, and A. Aspuru-Guzik. Atomistic study of the long-lived quantum coherences in the fenna-matthews-olson complex. *Biophys. J.*, 102:649, 2012.
- [14] M. Ceotto, **S. Valleau**, G. F. Tantardini, and A. Aspuru-Guzik. First principles semiclassical calculations of vibrational eigenfunctions. *J. Chem. Phys.*, 134:234103, 2011.

Teaching Experience

University of Washington <i>Chem E 545 - Data Science for Clean Energy Research</i> Graduate level class - Instructor	Seattle, UW Winter 2021
University of Washington <i>Chem E 465 - Reactor Design</i> Undergraduate level class - Instructor	Seattle, UW Fall 2020
University of Washington <i>Chem E 565 - Kinetics and Catalysis</i> Graduate level class - Instructor	Seattle, UW Winter 2020
University of Washington <i>Chem E 465 - Reactor Design</i> Undergraduate level class - Instructor	Seattle, UW Fall 2019
Harvard University <i>Quantum mechanics for physical chemistry</i> Graduate level class - Teaching Assistant. Responsibilities included holding sections, preparing and grading homework/exams and teaching some lectures.	Cambridge, MA Fall 2013
Harvard University <i>Physical sciences I</i> Undergraduate level class - Teaching Assistant. Responsibilities included holding bi-weekly sections and grading homework and exams.	Cambridge, MA Fall 2011
Harvard University <i>Physical sciences I</i> Undergraduate level class - Teaching Assistant. Responsibilities included holding bi-weekly sections and grading homework and exams. Also held interactive section for weaker students in the course.	Cambridge, MA Fall 2010

Professional Affiliation

American Institute of Chemical Engineers, AIChE, 2019-Current.
Computational Molecular Science and Engineering, CoMSEF, 2020-Current.
American Chemical Society, ACS, 2020-Current.

Professional Service

Service as Journal Reviewer: Physical Chemistry Chemical Physics, Physical Review Letters, The Journal of Physical Chemistry, The Journal of Physical Chemistry Letters, The Journal of Chemical Physics, New Journal of Physics, Philosophical Transactions of the Royal Society A, Journal of Computational Physics, Physical Review A., Physical Review Applied.

Service as Event Organizer:

- Creator and main organizer of Chemical Engineering Hackathon C-HACK, Department of Chemical Engineering, 2021-Current.

Service on Department Committees:

- Member of the Computing Infrastructure Committee, Department of Chemical Engineering, 2020-Current.
- Member of the Faculty Search Committee, Department of Chemical Engineering, 2020-Current.
- Member of the Data Science and Material Science Admissions and Operations Committee, Department of Chemical Engineering, 2020-Current.

- Member of the Graduate Admissions Committee, Department of Chemical Engineering, 2019-Current.
- Member of the Trainee Affairs Committee, Department of Chemical Engineering, 2019-Current.

Student Mentoring (primary advisor)

- Nida Janulaitis (PhD Student), 2019-present
- Evan Komp (PhD Student), 2019-present
- Brenden Pelkie (PhD Student), 2020-present
- Taner Yilmaz (BSc), 2019-2020

Student Awards and Honors

- John C. Berg endowed graduate fellowship, Brenden Pelkie (2020)
- Data Intensive Research Enabling Clean Technologies (DIRECT), Nida Janulaitis (2020)
- Data Intensive Research Enabling Clean Technologies (DIRECT), Evan Komp (2020)