

Stéphanie Valteau, Ph.D.

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Academic appointments

University of Washington
Assistant Professor

Seattle, WA
2019–Present

Education

Stanford University

Stanford, CA
2016–2019

Simons Foundation Postdoctoral Research Fellow

Simons Collaboration on the Origins of Life (SCOL)

SCOL Project: Atomistic exploration of abiogenesis with a nanoreactor.

Harvard University

Cambridge, MA

PhD in Physical Chemistry with Secondary Field in Computer Science

2010–2016

Dissertation title: Theoretical study of exciton transport in natural and synthetic light-harvesting systems.

Harvard University

Cambridge, MA

Master's of Arts (AM) in Physics

2013

Università degli Studi di Milano

Milan, Italy

Master's of Science in Physical Chemistry

2008–2010

Honors degree with grade 110/110 *Cum Laude*

Thesis title: A Quantum Instanton study of the diffusion of hydrogen and its isotopes on Ni(100).

Università degli Studi di Milano

Milan, Italy

Bachelor's of Science in Chemistry

2005–2008

Honors Degree with grade 110/100 *Cum Laude*

Thesis title: Quantum dynamics of the diffusion of hydrogen and its isotopes on Ni(100).

Awards & Fellowships

Simons Collaboration on the Origins of Life postdoctoral fellowship

Stanford University

Simons Foundation postdoctoral fellowship

2016

World-wide competition for a three-year postdoctoral fellowship from the Simons Collaboration on the Origins of Life.

ACS award in Computational Physical Chemistry

Harvard University

Graduate student award

2013

Nation-wide competition among graduate students in theoretical and computational chemistry, award includes 100K hours of computational time on the Blue Waters supercomputer.

Martin Karplus award

Harvard University

Graduate student award

2010

Professional service

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.

Conference Presentations

- S. Valleau**, *Poster*: Reaction dynamics of cyanohydrins 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] **S. Valleau** and T. J. Martínez. Reaction dynamics of cyanohydrins with hydrosulfide in water. *J. Phys. Chem. A.*, 123:7210–7217, 2019.
- [2] **S. Valleau** and T. J. Martínez. Reaction dynamics of cyanohydrins with hydrosulfide in water. *arXiv:1806.08841*, 2018.

- [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. *ACSNano*, 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

Seattle, UW

Instructor - undergraduate level class: Chem E 465 - Kinetics and Reaction Engineering

Fall 2019

Harvard University

Cambridge, MA

Teaching Assistant - graduate level class: Quantum mechanics for physical chemistry

Fall 2013

Responsibilities included holding sections, preparing and grading homework/exams and teaching some lectures.

Harvard University

Cambridge, MA

Teaching Assistant - undergraduate level class: Physical sciences I

Fall 2011

Responsibilities included holding bi-weekly sections and grading homework and exams.

Harvard University

Cambridge, MA

Teaching Assistant - undergraduate level class: Physical sciences I

Fall 2010

Responsibilities included holding bi-weekly sections and grading homework and exams. Also held interactive section for weaker students in the course.