Samuel M. Greene, Ph.D.

Computational materials science
Energy storage and conversion
Scientific software development

Oden Institute for Computational Engineering and Sciences
The University of Texas at Austin
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greenematerials.com

Education

2022 — PhD, Chemical Physics — Columbia University
Advisors: Timothy Berkelbach (Columbia), Jonathan Weare (NYU)
Dissertation: Stochastic Electronic Structure Methods for Molecules and Crystalline Solids

2016 — MSc by Research, Physical and Theoretical Chemistry — University of Oxford
Advisor: David Clary — Magdalen College

2014 — BS/MS, Chemistry — University of Chicago
GPA: 3.99 (honors)

Current Employment

2022 – present — **Postdoctoral Fellow, The University of Texas at Austin**
Oden Institute for Computational Engineering and Sciences
Advisor: Donald J. Siegel

- Performed atomistic simulations of materials for energy storage and conversion
- Predicted rates and mechanisms of ion transport in solid electrolytes for next-generation batteries using density functional theory and machine-learned interatomic potentials
- Predicted adsorption isotherms for water in metal-organic frameworks for thermal energy storage using machine-learned interatomic potentials and Monte Carlo sampling
- Contributed to 3 separate experimental collaborations
- Mentored 3 undergraduate students

This work resulted in 4 publications, including 1 first author (in *Chem. Mater.*) and was funded in part by Schmidt Science Fellows.

Fellowships and Awards

<u>International</u>

2022 — **Schmidt Science Fellows** (schmidtsciencefellows.org/)

- Supports PhD graduates who pivot into a different field for their postdoc
- 1 of 29 Fellows selected from 350 nominees in 2022
- Received 2 years of stipend support ($202,500)
- Attended scientific leadership training

2014 — **Rhodes Scholarship**

Last updated: September 16, 2025

National

2021 **DOE Office of Science Graduate Student Research Fellowship**
- Tuition and stipend support to conduct 1 year of PhD research at Berkeley Lab

2019 **Molecular Sciences Software Institute** (molssi.org)
- Received Seed (6-month) and Investment (18-month) Fellowships to support my PhD research (tuition and stipend support)

2016 Finalist, **Hertz Fellowship** (hertzfoundation.org/the-fellowship/)

2014 Finalist, **Marshall Scholarship**

2013 **Barry Goldwater Scholarship**
- Received 1 year of undergraduate tuition support

2013 **Phi Beta Kappa**

2012 Honorable mention, **Barry Goldwater Scholarship**

Institutional

2023 **Provost's Early Career Fellow**, The University of Texas at Austin
- Selected as 1 of 40 early-career scholars to receive targeted skills-development mentoring. Attended regular programming related to launching an academic career.

2022 **Pegram Award**, Department of Chemistry, Columbia University
- Received departmental award from the Columbia University Chemistry Department for outstanding students in the final year of their PhD

2018 **Gerhard Closs Teaching Award**, Department of Chemistry, U. of Chicago
- Yearly award for two Organic Chemistry TA's, chosen by the Lab Director on the basis of student evaluations

2017 **T. F. Cooke Teaching Award**, Department of Chemistry, Yale University
- Yearly award for three TA's, chosen on the basis of my student evaluations in General Chemistry and Honors General Chemistry

2014 **Francis E. Knock Prize**, Department of Chemistry, University of Chicago
- Awarded to outstanding graduating seniors

Computing resources for research

2024 **National Science Foundation ACCESS**
- Applied for (as the PI) and received 750,000 NSF ACCESS credits

Texas Advanced Computing Center (TACC)
- Applied for (as the PI) and received 500 node-hours

2023 **Texas Advanced Computing Center (TACC)**
- Applied for (as the PI) and received 2500 node-hours

2023 **National Science Foundation ACCESS**
- Applied for (as the PI) and received 750,000 NSF ACCESS credits

Publications

2024

K. Sada, S. M. Greene, S. Kmiec, D. J. Siegel, A. Manthiram. Unveiling the Influence of Water Molecules on the Structural Dynamics of Prussian Blue Analogues. *Small.* 20, 2406853. DOI: 10.1002/smll.202406853

S. M. Greene and D. J. Siegel. Assessing Correlations Between Phonon Features and Cation Migration Barriers in Multivalent Solid Electrolytes. *Chem. Mater.* 36, 7476-7486. DOI: 10.1021/acs.chemmater.4c01468

S. M. Greene, S. R. Schachat, N. Arita-Merino, X. E. Cao, H. Gurnani, M. Heyns, M. L. Cagigas, C. L. Maikawa, E. J. Needham, E. A. Perets, E. Phillips, A. W. Waddle, C. E. Wilkinson, K. C. Zhou, and H. M. Zlotnick. Accessible interview practices for disabled scientists and engineers. *iScience* 27, 110220. DOI: 10.1016/j.isci.2024.110220

J. S. Yoon, D. W. Liao, S. M. Greene, T. H. Cho, N. P. Dasgupta, and D. J. Siegel. Thermodynamics, Adhesion, and Wetting at Li/Cu(-Oxide) Interfaces: Relevance for Anode-Free Lithium–Metal Batteries. *ACS Appl. Mater. Interfaces* 16, 18790. DOI: 10.1021/acsami.3c19034

2023

H. Hao, Y. Liu, S. M. Greene, G. Yang, K. G. Naik, B. S. Vishnugopi, Y. Wang, H. Celio, A. Dolocan, W.-Y. Tsai, R. Fang, J. Watt, P. P. Mukherjee, D. J. Siegel, and D. Mitlin. Tuned Reactivity at the Lithium Metal–Argyrodite Solid State Electrolyte Interphase. *Adv. Energy Mater.,* 2301338. DOI: 10.1002/aenm.202301338

2022

S. M. Greene, R. J. Webber, J. E. T. Smith, J. Weare, and T. C. Berkelbach. Full Configuration Interaction Excited-State Energies in Large Active Spaces from Randomized Subspace Iteration. *J. Chem. Theory Comput.* 18, 7218-7232. DOI: 10.1021/acs.jctc.2c00435

S. M. Greene, R. J. Webber, T. C. Berkelbach, and J. Weare. Approximating Matrix Eigenvalues by Subspace Iteration with Repeated Random Sparsification. *SIAM J. Sci. Comput.* 44, A3067-A3097. DOI: 10.1137/21M1422513

2021

D. W. Laorenza, A. Kairalapova, S. L. Bayliss, T. Goldzak, S. M. Greene, L. R. Weiss, P. Deb, P. J. Mintun, K. A. Collins, D. D. Awschalom, T. C. Berkelbach, and D. E. Freedman. Tunable Cr^{4+} Molecular Color Centers. *J. Am. Chem. Soc.* 143, 21350–21363. DOI: 10.1021/jacs.1c10145

Y. Cho, S. M. Greene, and T. C. Berkelbach. Simulations of Trions and Biexcitons in Layered Hybrid Organic-Inorganic Lead Halide Perovskites. *Phys. Rev. Lett.* 126, 216402. DOI: 10.1103/PhysRevLett.126.216402

2020

S. M. Greene, R. J. Webber, J. Weare, and T. C. Berkelbach. Improved Fast Randomized Iteration Approach to Full Configuration Interaction. *J. Chem. Theory Comput.* 16, 5572–5585. DOI: 10.1021/acs.jctc.0c00437

K. Martinez-Cruz, A. Sepulveda-Jauregui, S. M. Greene, A. Fuchs, M. Rodriguez, N. Pansch, T. Gonsiorczyk, and P. Casper. Diel variation of CH_4 and CO_2 dynamics in two contrasting temperate lakes. *Inland Waters* 10, 333–347. DOI: 10.1080/20442041.2020.1728178

2019 S. M. Greene, R. J. Webber, J. Weare, and T. C. Berkelbach. Beyond Walkers in Stochastic Quantum Chemistry: Reducing Error Using Fast Randomized Iteration. *J. Chem. Theory Comput.* 15, 4834–4850. DOI: 10.1021/acs.jctc.9b00422

2018 S. M. Greene, X. Shan, and D. C. Clary. Quantum Scattering and Semiclassical Transition State Theory Calculations on Chemical Reactions of Polyatomic Molecules in Reduced Dimensions. *Adv. Chem. Phys.* 163, 117–150. DOI: 10.1002/9781119374978.ch4

2017 S. M. Greene and V. S. Batista. Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Method: Multidimensional Nonadiabatic Quantum Dynamics. *J. Chem. Theory Comput.* 13, 4034–4042. DOI: 10.1021/acs.jctc.7b00608

2016 S. M. Greene, X. Shan, and D. C. Clary. Rate constants of chemical reactions from semiclassical transition state theory in full and one dimension. *J. Chem. Phys.* 144, 244116. DOI: 10.1063/1.4954840

S. M. Greene, X. Shan, and D. C. Clary. An investigation of one- versus two-dimensional semiclassical transition state theory for H atom abstraction and exchange reactions. *J. Chem. Phys.* 144, 084113. DOI: 10.1063/1.4942161

2015 S. M. Greene, X. Shan, and D. C. Clary. Reduced-Dimensionality Semiclassical Transition State Theory: Application to Hydrogen Atom Abstraction and Exchange Reactions of Hydrocarbons. *J. Phys. Chem. A* 119, 12015–12027. DOI: 10.1021/acs.jpca.5b04379

A. Sepulveda-Jauregui, K. M. Walter Anthony, K. Martinez-Cruz, S. Greene, and F. Thalasso. Methane and Carbon Dioxide Emissions from 40 Lakes along a North–South Latitudinal Transect in Alaska. *Biogeosciences* 12, 3197–3223. DOI: 10.5194/bg-12-3197-2015

2014 S. Greene, K. M. Walter Anthony, D. Archer, A. Sepulveda-Jauregui, and K. Martinez-Cruz. Modeling the Impediment of Methane Ebullition Bubbles by Seasonal Lake Ice. *Biogeosciences* 11, 6791–6811. DOI: 10.5194/bg-11-6791-2014

Previous Research Experience

2021 – 2022 **Graduate Research Fellow, Lawrence Berkeley National Laboratory**
Advisors: Jeffrey B. Neaton, Jack Deslippe

- Developed new methods within the time-dependent GW-BSE formalism to study linear and nonlinear optical processes in monolayer semiconductors with potential applications in solar water splitting
- Collaborated with researchers at The University of California at Berkeley

This work was supported by a U.S. Department of Energy Office of Science Graduate Student Research Fellowship.

2017 – 2022 **Graduate Research Fellow, Columbia University**
Department of Chemistry
Advisors: Timothy C. Berkelbach, Jonathan Weare

- Developed custom Monte Carlo sampling techniques to improve the accuracy of quantum Monte Carlo methods
- Developed the software package FRIES (github.com/sgreene8/FRIES), a parallel implementation of these quantum Monte Carlo methods
- Benchmarked these methods on small molecules with Hilbert spaces as large as 10^{25}; demonstrated accuracy at less computational cost than existing methods
- Performed CASSCF-NEVPT2 calculations for an experimental collaboration on molecular qubits with Danna Freedman's group at MIT

This work was supported in part by fellowships from the Molecular Sciences Software Institute and resulted in 6 publications, 4 of which were first author (*J. Chem. Theory Comput.* and *SIAM J. Sci. Comput.*).

2016 – 2017 **Graduate Research Fellow, Yale University**
Department of Chemistry
Advisor: Victor S. Batista

- Developed an approach based on low-rank tensor factorizations to reduce the cost of nonadiabatic quantum dynamics simulations, and applied it to study the S_1/S_2 interconversion dynamics of pyrazine after UV photoexcitation

This work resulted in 1 first-author publication (*J. Chem. Theory Comput.*).

2014 – 2016 **Graduate Student Researcher, University of Oxford**
Department of Chemistry
Advisor: David C. Clary

- Developed a semiclassical method for calculating the rates of polyatomic chemical reactions from first principles and applied it to gas-phase H atom abstraction and exchange reactions

This work resulted in 4 first-author publications (*J. Phys. Chem. A*, *J. Chem. Phys.*, *Adv. Chem. Phys.*) and was supported by a Rhodes Scholarship.

2012 – 2014 **Undergraduate Student Researcher, University of Chicago**
Department of Geophysical Sciences
Advsiors: David Archer, Katey M. Walter Anthony

- Developed a semiempirical computer model for quantifying greenhouse gas emissions from thaw lakes in permafrost in Alaska
- Collaborated with researchers at The University of Alaska at Fairbanks

This work resulted in 3 publications, one of which was first author (*Biogeosciences*).

Summer 2013 **Jeff Metcalf Intern, New Brunswick Laboratory, U.S. Department of Energy**
Advisor: Michael Soriano

- Developed computational tools for calculating uncertainties in spectroscopic measurements of radioactive materials

Summer 2011 **REU Participant, Colorado School of Mines**
Department of Chemistry
Advisor: Ryan M. Richards

- Synthesized and characterized a catalyst for upgrading pyrolysis oil to biofuel

This work was supported by the NSF-funded Colorado Center for Biorefining and Biofuels through their research experience for undergraduates (REU) program.

Career Development Experiences

2024 **Auburn University's Preparing Future Faculty Workshop Series**

- Received coaching to prepare for the process of applying to faculty positions.

Presentations

Invited Talks

2019 S. M. Greene, R. J. Webber, J. Weare, T. C. Berkelbach. Randomized Electronic Structure Methods for Strongly Correlated Systems. National Renewable Energy Laboratory, Golden, CO.

2014 S. M. Greene. Keynote address to the graduating class of the Speech-Language Pathology master's program. University of Wisconsin, Madison, WI.

2012 S. M. Greene. Address to students about my experiences living with cerebral Palsy (in Chinese), *Changning* Primary Vocational Technical School, Shanghai, China.

Talks

2025 S. M. Greene, R. Randhar, and D. J. Siegel. Designing Metal-Organic Frameworks for Water Adsorption using Monte Carlo and Machine Learning Interatomic Potentials. MRS Spring Meeting and Exhibit, Seattle, WA

2024 S. M. Greene and D. J. Siegel. Computational Investigations of Features for Predicting Ionic Conductivity in Multivalent Solid Electrolytes. MRS Fall Meeting and Exhibit, Boston, MA.

S. M. Greene and D. J. Siegel. Computational Investigations of Features for Predicting Ionic Conductivity in Multivalent Solid Electrolytes. ECS PRiME 2024, Honolulu, HI.

S. M. Greene and D. J. Siegel. Predicting Ion Migration Barriers in Multivalent Solid Electrolytes from Phonon Features. Materials Discovery Seminar, Oden Institute for Computational Engineering and Sciences, Austin, TX.

S. M. Greene and D. J. Siegel. Predicting Ion Migration Barriers in Multivalent Solid Electrolytes from Phonon Features. Interfacial Chemistry and Charge Transfer for Energy Storage and Conversion, Telluride, CO.

S. M. Greene, S. R. Schachat, N. Arita-Merino, X. E. Cao, H. Gurnani, M. Heyns, M. L. Cagigas, C. L. Maikawa, E. J. Needham, E. A. Perets, E. Phillips, A. W. Waddle, C. E. Wilkinson, K. C. Zhou, H. M. Zlotnick. Universal Design Principles for Interviews in Science and Engineering. SciAccess Conference (virtual).

2024 S. M. Greene and D. J. Siegel. Predicting Ion Migration Barriers in Multivalent Solid Electrolytes from Phonons. MRS Spring Meeting and Exhibit, Seattle, WA.

2021 S. M. Greene, R. J. Webber, T. C. Berkelbach, L.-H. Lim, J. Weare. Fast Randomized Iteration for Full Configuration Interaction. SIAM Conference on Mathematical Aspects of Materials Science (virtual).

2013 S. M. Greene, A. Sepulveda-Jauregui, K. Martinez-Cruz K. M. Walter Anthony, and D. Archer. Entrapment of CH_4 Ebullition by Lake Ice. Workshop on Methane Dynamics in Arctic Ecosystems, University of Alaska, Fairbanks, AK.

Poster Presentations

2024 S. M. Greene, S. R. Schachat, N. Arita-Merino, X. E. Cao, H. Gurnani, M. Heyns, M. L. Cagigas, C. L. Maikawa, E. J. Needham, E. A. Perets, E. Phillips, A. W. Waddle, C. E. Wilkinson, K. C. Zhou, and H. M. Zlotnick. Accessible interview practices for disabled scientists and engineers. National Postdoc Appreciation Week Research Symposium, Austin, TX.

S. M. Greene and D. J. Siegel. Correlating Phonon Features and Cation Migration Barriers in Multivalent Solid Electrolytes. Gordon Research Conference on Batteries, Ventura, CA.

2023 S. M. Greene and D. J. Siegel. Computational Screening of Metal-Organic Frameworks for Thermal Energy Storage. Rhodes 120th Anniversary Reunion, Oxford, UK.

2021 S. M. Greene, R. J. Webber, T. C. Berkelbach, J. Weare. Full Configuration Interaction Excited States from Fast Randomized Iteration. TSRC Workshop on Stochastic Methods in Electronic Structure Theory (virtual).

2018 S. M. Greene, R. J. Webber, J. Weare, T. C. Berkelbach. Randomized Iterative Methods for Electronic Structure Calculations. Midwest Theoretical Chemistry Conference, Chicago, IL. (**Received poster award**)

2017 S. M. Greene and V.S. Batista. The TT-SOFT Method: An Efficient Approach to High-Dimensional Quantum Dynamics Simulations Based on Tensor-Train Decomposition. American Conference on Theoretical Chemistry, Boston, MA.

S. M. Greene and V.S. Batista. The TT-SOFT Method: An Efficient Approach to High-Dimensional Quantum Dynamics Simulations Based on Tensor-Train Decomposition. Machine Learning for Materials Research Bootcamp, College Park, MD.

Teaching Experience

Spring 2018 **Teaching Assistant, University of Chicago**
Chemical Kinetics and Dynamics
Department of Chemistry

- Held office hours and graded assignments and exams for 27 undergraduate students

Winter 2018
Fall 2017

Teaching Assistant, University of Chicago
Organic Chemistry
Department of Chemistry

- Led discussion sections, supervised labs, held office hours, and graded homework assignments and exams for 14 undergraduate students per quarter
- Wrote practice questions to foster an environment of open problem solving and discussion
- Set up an online forum to allow students to ask questions asynchronously

Spring 2017

Teaching Fellow, Yale University
Honors General Chemistry
Department of Chemistry

- Led discussion sections, held office hours, wrote homework questions, and graded homework assignments and exams for 22 undergraduate students

Fall 2016

Teaching Fellow, Yale University
General Chemistry
Department of Chemistry

- Led discussion sections, held office hours, wrote homework questions, and graded exams for 23 undergraduate students
- Led problem-solving sessions for students to work through practice problems with peers
- Organized extra exam review sessions

Summer 2015

Full-time Teacher, Oxbridge Academic Programs
Computer Science and App Design

- Developed the curriculum and taught 2 sections of 23 international students in grades 8 and 9
- Graded homework and quizzes
- Developed and supervised interactive computer programming exercises

Spring 2014
Fall 2013

Teaching Assistant, University of Chicago
Global Warming: The Science and Modeling of Climate Change
(coursera.org/learn/global-warming)
Department of the Geophysical Sciences

- Developed quiz questions and computer modeling activities for two iterations of an online course with 10,000+ students
- Monitored discussion forums and answered questions

Research Mentoring Experience

2024 – present

Rushil Randhar, Undergraduate student (Computational Engineering and Plan II Honors), The University of Texas at Austin

2024 – present

Rushil Randhar, Undergraduate student (Computational Engineering and Plan II Honors), The University of Texas at Austin

2024 – present

Olivia Castillo, Undergraduate student (Physics Honors and Plan II Honors), The University of Texas at Austin

Academic Service

2024 – present **Member, Rhodes and Marshall Selection Committee**
The University of Texas at Austin

- Read applications, conducted interviews, and participated in the selection of campus nominees for the Rhodes and Marshall Scholarships

2023 – present **Reviewer**, *Journal of Chemical Theory and Computation*

2021 – present **Mentor, Goldwater Scholarship Community**

- Provided one-on-one mentoring to undergraduate Goldwater Scholars on graduate school, scientific research, and British fellowship applications
- Presented at online webinars on graduate school and fellowship applications

2022 **Member, Rhodes Scholarship Selection Committee**
U.S. District 6

- Read applications, selected finalists, performed interviews, selected Rhodes Scholars

2017 – 2018 **Volunteer Interviewer, College Center for Research and Fellowships**
The University of Chicago

- Read applications and performed mock interviews for British fellowship finalists

2016 **Volunteer Interviewer, Fellowships and Funding**
Yale University

- Read applications and performed mock interviews for Rhodes Scholarship finalists

2015 – 2016 **Reviewer**, *Chemical Physics Letters*

Professional Experience

2012 **Software Development Intern, Increpreneur** (start-up in Shanghai, China)

- Developed a JavaScript library for web developers to collect user feedback