Evan Spotte-Smith, PhD

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Evan Walter Clark Spotte-Smith (they/them/their)
Computational and Data Chemist

Education

2019–2023	**Doctor of Philosophy**, *University of California, Berkeley (UC Berkeley).*
	Materials Science and Engineering
	Advisor: Professor Kristin Persson
	Thesis: "On the Exploration of Electrochemical Reaction Cascades"
2019–2021	**Master of Science**, *UC Berkeley.*
	Materials Science and Engineering
2015–2019	**Bachelor of Science**, *Columbia University.*
	Major: Materials Science and Engineering
	Minor: Sustainable Engineering

Research

2025 –	**(Incoming) Assistant Professor, Chemical Engineering**, *Carnegie Mellon University (CMU).*
2024 –	**Carnegie Bosch Institute Fellow**, *CMU.*
2024	**Postdoctoral Fellow, Gomes Group**, *CMU.*
2019 – 2023	**Graduate Student Researcher, Persson Group**, *Lawrence Berkeley National Laboratory (LBNL).*
2023	**Cell Modeling Intern**, *Tesla Motors.*
2018 – 2019	**Undergraduate Student Researcher, Hacking Materials Group**, *LBNL.*
2016 – 2019	**Lead Undergraduate Researcher, Herman Group**, *Columbia University.*

Teaching

2022	**Graduate Student Instructor**, *UC Berkeley Department of Chemistry.*
	General Chemistry and Quantitative Analysis
	Evaluation: median 7.0/7.0; mean 6.5/7.0
2020	**Instructor**, *Materials Project Workshop 2020.*
	Pymatgen Foundations
2018	**Course Assistant**, *Columbia University Department of Applied Physics and Applied Mathematics.*
	Thermodynamics, Kinetic Theory, and Statistical Mechanics

Mentorship

2022 – 2023	**Laura Zichi.**
	Project: Developing tools to simulate reactivity at dynamic fluid-solid interfaces
2021 – 2022	**Thea Petrocelli.**
	Project: Understanding salt decomposition in batteries from first principles
2021 – 2022	**Nikita Redkar.**
	Project: Learning electrochemical reaction products using natural language processing
2020 – 2022	**Aniruddh Khanwale.**
	Project: Calculation of charge transfer rates through battery interphases
2020 – 2021	**Ronald Kam.**
	Project: Kinetic modeling of lithium-ion solid-electrolyte interphase formation

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Honors & Awards

2024	**Carnegie Bosch Institute Fellowship**, CMU.
2024	**President's Postdoctoral Fellowship (declined)**, CMU.
2023	**Pre-faculty Workshop Participant**, NextProf Nexus.

2023	**1st Prize**, Winton-Kavli Research Pitch Competition.
2023	**1st Prize, Innovation Expo**, Berkeley Energy & Resource Collaborative Energy Summit.
2022	**Battery Student Slam Winner**, 241st Electrochemical Society Meeting.
2022	**Philomathia Graduate Student Fellowship**, Kavli Energy Nanoscience Institute.
2020	**Honorable Mention**, NSF Graduate Research Fellowship Program.
2019	**Honorable Mention**, NSF Graduate Research Fellowship Program.
2019	**Frank McQuiston Fellowship**, UC Berkeley Department of Materials Science and Engineering.
2019	**Clarendon Fund Scholarship (declined)**, University of Oxford.
2019	*Magna Cum Laude*, Columbia University.
2019	**Tau Beta Pi New York Alpha Chapter**.
2019	**Francis B. F. Rhodes Prize**, Columbia University.
2019	**King's Crown Leadership Excellence Award for Civic Responsibility**, Columbia University.

Resources & Funding

2024 – 2025 **Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS)**, *National Science Foundation.*
Project: Rational Design of Electrolytes for Ammonia Synthesis Using Machine-Learned Potentials
Award type: High-performance computing allocation
Role: Lead PI
Total award amount: 750,000 ACCESS credits

2024 – 2026 **Synthesis Advanced Research Challenge**, *Toyota Research Institute.*
Project: Direct Introduction of Competition and Kinetics to Materials Mechanism and Reaction Network Prediction
Award type: Funding
Role: Lead PI
Total award amount: $500,000

2020 – 2024 **Schrodinger, Inc.**.
Award type: Partnership
Role: Initiated partnership, lead point of contact
Total award amount: In kind, valued at $5,517,000

2021 – 2024 **High-Performance Computing**, National Renewable Energy Laboratory.
Project: Integrated Modeling and Machine Learning of Solid-Electrolyte Interface Reactions of the Si Anode
Award type: High-performance computing allocation
Role: Contributor
Total award amount: 6,884,000 node-hours

2020 – 2023 **Energy Research Computing Allocations Process (ERCAP)**, National Energy Research Supercomputing Center (NERSC).
Award type: High-performance computing allocation
Role: Contributor
Total award amount: 325,000 node-hours

Peer-Reviewed Publications

(Note: * = Equal Contribution)

[1] Mel Soto, Kae Fink, Christof Zweifel, Peter J. Weddle, **Evan Walter Clark Spotte-Smith**, Gabriel M. Veith, Kristin A. Persson, Andrew M. Colclasure, and Bertrand J. Tremolet de Villers. Solubilities of ethylene and carbon dioxide gases in lithium-ion battery electrolyte. *Journal of Chemical & Engineering Data*, 2024.

[2] Noel J. Leon, Stefan Illic, Xiaowei Xie, Heonjae Jeong, Zhenzhen Yang, Bingning Wang, **Evan Walter Clark Spotte-Smith**, Charlotte Stern, Nathan Hahn, Kevin Zavadil, Lei Cheng, Kristin Persson, Justin Connell, and Chen Liao. Achieving new calcium alkoxyaluminate salts with a novel synthetic route. *The Journal of Physical Chemistry Letters*, 15(19):5096–5102, 2024.

[3] Sudarshan Vijay, Maxwell Venetos, **Evan Walter Clark Spotte-Smith**, Aaron Kaplan, Mingjian Wen, and Kristin A. Persson. CoeffNet: Predicting activation barriers through a constrained, equivariant and chemically-interpretable graph neural network. *Chemical Science*, 15(8):2923–2936, 2024.

[4]   **Evan Walter Clark Spotte-Smith***, Sudarshan Vijay*, Thea Bee Petrocelli, Bernardine L. D. Rinkel, Bryan D. McCloskey, and Kristin A. Persson. A critical analysis of chemical and electrochemical oxidation mechanisms in Li-ion batteries. *The Journal of Physical Chemistry Letters*, 15(2):391–400, 2024.

[5]   Rishabh D. Guha*, Santiago Vargas*, **Evan Walter Clark Spotte-Smith**, Alexander Rizzolo Epstein, Maxwell Venetos, Mingjian Wen, Ryan Kingsbury, Samuel M. Blau, and Kristin A. Persson. HEPOM: A predictive framework for accelerated hydrolysis energy predictions of organic molecules. *NeurIPS AI4Mat*, 2023.

[6]   **Evan Walter Clark Spotte-Smith**, Orion Archer Cohen, Samuel M. Blau, Jason M. Munro, Ruoxi Yang, Rishabh D. Guha, Hetal D. Patel, Sudarshan Vijay, Patrick Huck, Ryan Kingsbury, Matthew K. Horton, and Kristin A. Persson. A database of molecular properties integrated in the Materials Project. *Digital Discovery*, 2(6):1862–1882, 2023.

[7]   Peter J. Weddle, **Evan Walter Clark Spotte-Smith**, Ankit Verma, Hetal D. Patel, Kae Fink, Bertrand J. Tremolet de Villers, Maxwell C. Schulze, Samuel M. Blau, Kandler A. Smith, Kristin A. Persson, and Andrew M. Colclasure. Continuum-level modeling of Li-ion battery SEI by upscaling atomistically informed reaction mechanisms. *Electrochimica Acta*, 468(143121), 2023.

[8]   **Evan Walter Clark Spotte-Smith**, Samuel M. Blau, Daniel Barter, Noel J. Leon, Nathan T. Hahn, Nikita S. Redkar, Kevin R. Zavadil, Chen Liao, and Kristin A. Persson. Chemical reaction networks explain gas evolution mechanisms in Mg-ion batteries. *Journal of the American Chemical Society*, 145(22):12181–12192, 2023.

[9]   **Evan Walter Clark Spotte-Smith***, Alexander Rizzolo Epstein*, Maxwell Venetos, Oxana Andriuc, and Kristin A. Persson. Assessing the accuracy of density functional approximations for predicting hydrolysis reaction kinetics. *Journal of Chemical Theory and Computation*, 19(11):3159–3171, 2023.

[10]   Mingjian Wen, **Evan Walter Clark Spotte-Smith**, Samuel M. Blau, Matthew J. McDermott, Aditi Krishnapriyan, and Kristin A. Persson. Chemical reaction networks and opportunities for machine learning. *Nature Computational Science*, 3:12–24, 2023.

[11]   **Evan Walter Clark Spotte-Smith***, Daniel Barter*, Nikita S. Redkar, Aniruddh Khanwale, Shyam Dwaraknath, Kristin A. Persson, and Samuel M. Blau. Predictive stochastic analysis of massive filter-based electrochemical reaction networks. *Digital Discovery*, 2(123):123–137, 2023.

[12]   **Evan Walter Clark Spotte-Smith***, Thea Bee Petrocelli*, Hetal D. Patel, Samuel M. Blau, and Kristin A. Persson. Elementary decomposition mechanisms of lithium hexafluorophosphate in battery electrolytes and interphases. *ACS Energy Letters*, 8(1):347–355, 2023.

[13]   Xiaowei Xie, Noel J. Leon, David W. Small, **Evan Walter Clark Spotte-Smith**, Chen Liao, and Kristin A. Persson. The reductive decomposition kinetics and thermodynamics that govern the design of fluorinated alkoxyaluminate/borate salts for Mg-ion and Ca-ion batteries. *Journal of Physical Chemistry C*, 126(49):20773–20785, 2022.

[14]   **Evan Walter Clark Spotte-Smith***, Ronald Kam*, Daniel Barter, Xiaowei Xie, Tingzheng Hou, Shyam Dwaraknath, Samuel M. Blau, and Kristin A. Persson. Toward a mechanistic model of solid-electrolyte interphase formation and evolution in lithium-ion batteries. *ACS Energy Letters*, 7(4):1446–1453, 2022.

[15]   Lorena Alzate-Vargas, Samuel Blau, **Evan Walter Clark Spotte-Smith**, Srikanth Allu, Kristin A. Persson, and Jean-Luc Fattebert. Insight into SEI growth in Li-ion batteries using molecular dynamics and accelerated chemical reactions. *Journal of Physical Chemistry C*, 125(34):18588–18596, 2021.

[16]   Xiaowei Xie, **Evan Walter Clark Spotte-Smith**, Mingjian Wen, Hetal Patel, Samuel M. Blau, and Kristin A. Persson. Data-driven prediction of formation mechanisms of lithium ethylene monocarbonate with an automated reaction network. *Journal of the American Chemical Society*, 143(33):13245–13258, 2021.

[17]   **Evan Walter Clark Spotte-Smith***, Samuel M. Blau*, Xiaowei Xie, Hetal D. Patel, Mingjian Wen, Brandon Wood, Shyam Dwaraknath, and Kristin A. Persson. Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. *Scientific Data*, 8(203), 2021.

[18] Samuel M. Blau, Hetal Patel, **Evan Walter Clark Spotte-Smith**, Xiaowei Xie, Shyam Dwaraknath, and Kristin A. Persson. A chemically consistent graph architecture for massive reaction networks applied to solid-electrolyte interphase formation. *Chemical Science*, 12(13):4931–4939, 2021.

[19] Mingjian Wen, Samuel M. Blau, **Evan Walter Clark Spotte-Smith**, Shyam Dwaraknath, and Kristin A. Persson. BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules. *Chemical Science*, 12(5):1858–1868, 2021.

[20] Jiayang Hu, **Evan Walter Clark Spotte-Smith**, Brady Pan, Roy Garcia, Carlos Colosqui, and Irving P Herman. Spatiotemporal study of iron oxide nanoparticle monolayer formation at liquid/liquid interfaces by using in-situ small angle x-ray scattering. *The Journal of Physical Chemistry C*, 124(13):23949–23963, 2020.

[21] **Evan Walter Clark Spotte-Smith**, Peiyuan Yu, Samuel M. Blau, Anubhav Jain, and Ravi S. Prasher. Aqueous Diels-Alder reactions for thermochemical storage and heat transfer fluids identified using density functional theory. *Journal of Computational Chemistry*, 41(24):2137–2150, 2020.

[22] Jiayang Hu, **Evan Walter Clark Spotte-Smith**, Brady Pan, and Irving P. Herman. Improved small-angle x-ray scattering of nanoparticle self-assembly using a cell with a flat liquid surface. *Journal of Nanoparticle Research*, 21(4):71, 2019.

Other Publications

[1] Eric Sivonxay, Lucas Attia, **Evan Walter Clark Spotte-Smith**, Benjamin Sanchez-Lengeling, Xiaojing Xia, Daniel Barter, Emory M. Chan, and Samuel M. Blau. Inverse design of complex nanoparticle heterostructures via deep learning on heterogeneous graphs. In preparation, 2024.

[2] **Evan Walter Clark Spotte-Smith**, Kareem Hegazy, Matthew Avaylon, Santiago Vargas, Orion A. Cohen, Michael W. Mahoney, Talita Perciano, Kristin A. Persson, and Samuel M. Blau. Calculated properties of molecules at diverse charge and spin states for next-generation chemical machine learning. In preparation, 2024.

[3] Robert MacKnight, Daniil A. Boiko, **Evan Walter Clark Spotte-Smith**, Jose Emilio Regio, Liliana C. Gallegos, ThÃlo A. Neukomm, and Gabriel dos Passos Gomes. Opportunities and challenges for large language models in the chemical sciences. In review, 2024.

[4] Matthew K. Horton, Patrick Huck, Ruoxi X. Yang, Jason M. Munro, Shyam Dwaraknath, Alexander M. Ganose, Ryan S. Kingsbury, Mingjian Wen, Jimmy-Xuan Shen, Tyler S. Mathis, Aaron D. Kaplan, Karlo Berket, Janosh Riebesell, Janine George, Andrew S. Rosen, **Evan Walter Clark Spotte-Smith**, Matthew J. McDermott, Orion A. Cohen, Alexander Dunn, Matthew Kuner, Gian-Marco Rignanese, Geoffrey Hautier, Guido Petretto, David Waroquiers, Sinead M. Griffin, Jeffrey B. Neaton, Daryl C. Chrzan, Mark Asta, Shreyas Cholia, Gerbrand Ceder, Shyue Ping Ong, Anubhav Jain, and Kristin A. Persson. The materials project: A decade of materials discovery. In review, 2024.

[5] Laura Zichi*, Daniel Barter*, Eric Sivonxay*, **Evan Walter Clark Spotte-Smith**, M. Rohith Srinivaas, , Emory Chan, Kristin A. Persson, and Samuel M. Blau. RNMC: kinetic Monte Carlo implementations for complex reaction networks. In review, 2024.

[6] Samuel Blau*, **Evan Walter Clark Spotte-Smith***, Brandon Wood, Shyam Dwaraknath, and Kristin Persson. Accurate, automated density functional theory for complex molecules using on-the-fly error correction. *ChemRxiv*, DOI:10.26434/chemrxiv.13076030.v1, 2020.

Presentations

[1] **Evan Walter Clark Spotte-Smith**. Data-driven design of reactive technologies: Case studies in energy storage, 2025. ACS Spring Meeting (**Invited Talk**).

[2] **Evan Walter Clark Spotte-Smith**, Andrew Timmins, and Rachel C. Kurchin. Mechanistic insights into electrolyte decomposition during electrochemical ammonia synthesis from machine-learning interatomic potentials, 2025. ACS Spring Meeting.

[3] **Evan Walter Clark Spotte-Smith**. Chemical reaction network machine learning (CRN-ML): A frontier for reactivity studies, 2024. AIMED Workshop on Heterogeneous Catalysis (**Invited Poster**).

[4] **Evan Walter Clark Spotte-Smith**. Datasets to drive practical chemical data science, 2024. Gordon Research Conference in Computational Chemistry.

[5] **Evan Walter Clark Spotte-Smith**, Kareem Hegazy, Matthew Avaylon, Santiago Vargas, Orion A. Cohen, Michael W. Mahoney, Talita Perciano, Kristin A. Persson, and Samuel M. Blau. Challenging molecular machine learning with datasets of ions and radicals, 2024. Gordon Research Seminar in Computational Chemistry (**Invited Talk**).

[6] **Evan Walter Clark Spotte-Smith**. Using networks to obtain mechanistic understanding in electrochemistry, 2024. Materials Science and Engineering Rising Stars Colloquium Series (**Invited Talk**).

[7] **Evan Walter Clark Spotte-Smith**. Rational design of sustainable chemical solutions with reaction networks and data science, 2023. AIChE Annual Meeting.

[8] **Evan Walter Clark Spotte-Smith**, Samuel M. Blau, Daniel Barter, Noel J. Leon, Nathan T. Hahn, Nikita S. Redkar, Kevin R. Zavadil, Chen Liao, and Kristin A. Persson. Explaining gas evolution mechanisms in Mg-ion batteries with chemical reaction networks, 2023. AIChE Annual Meeting.

[9] **Evan Walter Clark Spotte-Smith**, Orion Cohen, Samuel M. Blau, Jason M. Munro, Ryan Kingsbury, Rishabh D. Guha, Hetal D. Patel, Sudarshan Vijay, Ruoxi Yang, Patrick Huck, Matthew K. Horton, and Kristin A. Persson. MPcules: an open and accessible database of molecular properties in the Materials Project, 2023. ACS Fall Meeting.

[10] **Evan Walter Clark Spotte-Smith**, Thea Bee Petrocelli, Hetal D. Patel, Samuel M. Blau, and Kristin A. Persson. Revealing the decomposition mechanisms of lithium hexafluorophosphate in battery electrolytes and interphases by first-principles simulations, 2023. ACS Spring Meeting.

[11] **Evan Walter Clark Spotte-Smith**, Daniel Barter, Ronald L. Kam, Chen Liao, Samuel M. Blau, and Kristin A. Persson. Explaining battery electrolyte decomposition with chemical reaction networks, 2023. Berkeley Energy & Resources Collaborative Energy Summit.

[12] **Evan Walter Clark Spotte-Smith**. Leveraging quantum chemistry and reaction networks to explore electrochemical cascades, 2022. Pitzer Center for Theoretical Chemistry Seminar Series.

[13] **Evan Walter Clark Spotte-Smith**. Leveraging big data and chemical reaction networks to explore and explain electrochemistry, 2022. ChemE Future Faculty Seminar Series.

[14] **Evan Walter Clark Spotte-Smith**, Ronald L. Kam, Daniel Barter, Julian Self, Xiaowei Xie, Tingzheng Hou, Shyam Dwaraknath, Samuel M. Blau, and Kristin A. Persson. A general mechanistic model of early solid-electrolyte interphase formation in lithium-ion batteries, 2022. Gordon Research Conference in Electrochemistry.

[15] **Evan Walter Clark Spotte-Smith**, Ronald L. Kam, Daniel Barter, Xiaowei Xie, Tingzheng Hou, Shyam Dwaraknath, Samuel M. Blau, and Kristin A. Persson. Towards a mechanistic explanation for solid electrolyte interphase formation and evolution in lithium-ion batteries, 2022. American Conference on Theoretical Chemistry.

[16] **Evan Walter Clark Spotte-Smith**, Ronald L. Kam, Daniel Barter, Xiaowei Xie, Tingzheng Hou, Shyam Dwaraknath, Samuel M. Blau, and Kristin A. Persson. Towards a mechanistic explanation for solid electrolyte interphase formation and evolution in lithium-ion batteries, 2022. 21st International Meeting on Lithium Batteries (**Invited Poster**).

[17] **Evan Walter Clark Spotte-Smith**, Ronald L. Kam, Daniel Barter, Julian Self, Xiaowei Xie, Tingzheng Hou, Shyam Dwaraknath, Samuel M. Blau, and Kristin A. Persson. Towards a mechanistic explanation for solid electrolyte interphase formation in lithium-ion batteries, 2022. 241st Electrochemical Society Meeting.

[18] **Evan Walter Clark Spotte-Smith**, Samuel M. Blau, and Kristin A. Persson. GPS for the SEI: Charting electrochemical mechanisms with reaction networks, 2022. 241st Electrochemical Society Meeting.

[19] **Evan Walter Clark Spotte-Smith**, Samuel M. Blau, Xiaowei Xie, Brandon Wood, Hetal Patel, Shyam Dwaraknath, and Kristin A. Persson. Automatic generation of computational reaction networks for unbiased exploration of chemical pathways, 2020. 2020 MRS Spring/Fall Meeting & Exhibit.

[20] **Evan Walter Clark Spotte-Smith**, Samuel M. Blau, Brandon Wood, Shyam Dwaraknath, and Kristin A. Persson. A robust computational framework for high-throughput density functional theory calculations for electrochemical application, 2020. PRiME 2020 (ECS, ECSJ, & KECS Joint Meeting).

[21] **Evan Walter Clark Spotte-Smith**, Peiyuan Yu, Anubhav Jain, and Ravi Prasher. Identifying Diels-Alder reactions for aqueous thermal storage using density functional theory, 2019. 2019 MRS Spring Meeting and Exhibit.

Contributed Reviews

2024 *The Journal of Open Source Software* (x2), *Scientific Data*, *Digital Discovery*, *Journal of Physics D: Applied Physics*, *Journal of Chemical Theory and Computation*

2023 *ACS Nano*, *Journal of Chemical Information and Modeling*, *npj Computational Materials*

2022 *ACS Energy Letters*, *The Journal of Open Source Software*

Organized Symposia and Workshops

2025 **"Chemical reaction networks, retrosynthesis, and reaction prediction"**, ACS Fall Meeting

2023 **Kavli Career Development Workshop**, UC Berkeley

Leadership & Service

2022 – 2023 **UC Berkeley Graduate Assembly**.
- Advocate on behalf of materials science graduate students
- Develop policies and legislation to promote the well-being of UC Berkeley graduate students
- **Previous Roles**: Materials Science and Engineering Delegate

2020 – 2023 **UC Berkeley Materials Science and Engineering Graduate Student Council**.
- Advocate to department administration and faculty for issues of importance to graduate students
- Organize events to build community among materials science graduate students
- Coordinate anti-racist reading groups in collaboration with UC Berkeley College of Chemistry
- **Previous Roles**: Vice-President, Social Chair

2020 – 2021 **CalACS College Application and Professional Support (CAPS)**.
- Participate in weekly workshops with high school students to improve professional skills
- Develop long-term mentoring relationships with low-income, first-generation college applicants
- Provide one-on-one assistance for college and job applications
- **Previous Roles**: Mentor

2020, 2021 **Faculty Search Committee**, UC Berkeley Department of Materials Science and Engineering.
- Succeeded in hiring Xiaoyu (Rayne) Zheng for the position of Associate Professor

2020 **Interstitials Mentorship Program**.
- Led peer-to-peer mentorship program for materials science community
- **Previous Roles**: Co-Director

2015 – 2018 **Columbia University Engineers Without Borders (CU-EWB)**.
- Designed and implemented solar micro-grids for rural communities in the Teso Sub-Region of Uganda
- **Previous Roles**: Engineering Mentor, President, Program Manager, Director of Grants, Program Liaison, Director of Operations

2016 – 2018 **Columbia Educational Simulations (CESIMS)**.
- Trained 25 student delegates at The Brooklyn Latin School for local and regional debate conferences
- Led lessons and simulations on public speaking, history, and international affairs
- Mentored students in order to prepare them for college and careers
- **Previous Roles**: Academic Advisor