Evan Spotte-Smith

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

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Education

2019–2024	**Doctor of Philosophy**, *University of California, Berkeley (UC Berkeley).*
	Materials Science and Engineering
	Advisor: Professor Kristin Persson
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

2019 – 2024 Graduate Student Researcher, Persson Group, *Lawrence Berkeley National Laboratory (LBNL).*
- Construct and manage open datasets of molecular properties based on density functional theory (DFT)
- Design and implement methods to explore and analyze chemical reaction networks
- Explain electrolyte degradation, gas evolution, and interphase formation in Li-ion and Mg-ion batteries

2023 Cell Modeling Intern, *Tesla Motors.*
- Accelerated prediction of electrolyte transport properties through algorithmic optimization
- Evaluated electrolyte additives for high-voltage Li-ion cathodes and silicon anodes in terms of gas evolution and electrode passivation

2018 – 2019 Undergraduate Student Researcher, Hacking Materials Group, *LBNL.*
- Performed computational screening studies of Diels-Alder reactions for liquid-phase thermal energy storage
- Identified reactions leading to exceptional heat capacity enhancement in aqueous thermal fluids

2016 – 2019 Lead Undergraduate Researcher, Herman Group, *Columbia University.*
- Developed a sample cell architecture to improve small angle x-ray scattering signal from liquid interfaces
- Revealed an unexpected transport mechanism controlling nanoparticle self-assembly kinetics

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

Honors & Awards

Resources & Funding

Peer-Reviewed Publications

(Note: * = Equal Contribution)

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*, 2023.

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*, 2023.

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.

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), 2023.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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

(Note: * = Equal Contribution)

Evan Walter Clark Spotte-Smith, Samuel M. Blau, Santiago Vargas, Rishabh Guha, and Kristin A. Persson. Diverse datasets of elementary molecular reactions and related trajectories. *In preparation*, 2023.

Mel Soto, Peter J. Weddle, **Evan Walter Clark Spotte-Smith**, Kristin A. Persson, Kae Fink, and Bertrand J. Tremolet de Villers. Solubility of ethylene and carbon dioxide gas in battery electrolytes. *In preparation*, 2023.

Laura Zichi*, Daniel Barter*, Eric Sivonxay*, **Evan Walter Clark Spotte-Smith**, Rohith Srinivaas Mohanakrishnan, Kristin A. Persson, and Samuel M. Blau. RNMC: kinetic Monte Carlo implementations for complex reaction networks. *In preparation*, 2023.

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. *In preparation*, 2023.

Evan Walter Clark Spotte-Smith, Orion Cohen, Samuel M. Blau, Jason M. Munro, Ruoxi Yang, Rishabh Guha, Hetal D. Patel, Sudarshan Vijay, Patrick Huck, Ryan Kingsbury, Matthew K. Horton, and Kristin A. Persson. Rich and accessible molecular properties integrated in the Materials Project database. *In preparation*, 2023.

Peter J. Weddle, **Evan Walter Clark Spotte-Smith**, Ankit Verma, Hetal D. Patel, Kar 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. *In Review*, 2023.

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*, 2020. DOI:10.26434/chemrxiv.13076030.v1.

Posters & Presentations

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. ACS Fall Meeting, 2023.

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. ACS Spring Meeting, 2023.

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. Berkeley Energy & Resources Collaborative Energy Summit, 2023.

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

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

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. Gordon Research Conference in Electrochemistry, 2022.

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. American Conference on Theoretical Chemistry, 2022.

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. 21st International Meeting on Lithium Batteries (**Invited Poster**), 2022.

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. 241st Electrochemical Society Meeting, 2022.

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

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 MRS Spring/Fall Meeting & Exhibit, 2020.

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. PRiME 2020 (ECS, ECSJ, & KECS Joint Meeting), 2020.

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 MRS Spring Meeting and Exhibit, 2019.

Contributed Reviews

| 2023 | *ACS Nano, npj Computational Materials* |
| 2022 | *ACS Energy Letters, The Journal of Open Source Software* |

Leadership & Service

2022 – 2023 · **UC Berkeley Course Materials and Services Fees Committee**.
- Review policies related to fees for UC Berkeley courses
- Advise the Chancellor regarding appropriate costs and fees
- **Previous Roles**: Graduate Student Representative

2022 – 2023 · **Chancellor's Advisory Committee on the LGBTQ+ Communities at Cal**.
- Advise UC Berkeley administration on the needs of queer and trans members of the Berkeley community
- Evaluate campus and UC system policies as they relate to LGBTQ+ campus members
- **Previous Roles**: Graduate Student Representative

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 Assistant 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