

Evan Spotte-Smith

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

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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 – Present **Graduate Student Researcher, Persson Group**, *Lawrence Berkeley National Laboratory (LBNL)*.
 - Leverage density functional theory (DFT) calculations for machine learning of reaction properties
 - Develop methods to explore and analyze chemical reaction networks.
 - Explain the mechanistic origins of solid electrolyte interphase (SEI) formation in Li-ion and Mg-ion batteries.
- 2018 – 2019 **Undergraduate Student Researcher, Hacking Materials Group**, *LBNL*.
 - Performed computational screening studies of Diels-Alder reactions for liquid-phase thermal energy storage.
 - Using DFT, 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 dominant 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 – Present **Laura Zichi**.
Project: Microkinetic modeling of solid electrolyte interphase formation at long time scales
- 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

- 2022 **Battery Student Slam Winner**, 241st Electrochemical Society Meeting.
- 2022 **Philomathia Graduate Student Fellowship**, Kavli Energy Nanoscience Institute.
- 2019, 2020 **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

- 2020 - 2023 **Schrodinger, Inc..**
Award type: Partnership
Total award amount: In kind, valued at \$3,586,000
- 2021 - 2023 **High-Performance Computing**, National Renewable Energy Laboratory.
Project title: Integrated Modeling and Machine Learning of Solid-Electrolyte Interface Reactions of the Si Anode
Award type: High-performance computing allocation
Total award amount: 5,248,000 node-hours
- 2020 - 2023 **Energy Research Computing Allocations Process (ERCAP)**, National Energy Research Supercomputing Center (NERSC).
Award type: High-performance computing allocation
Total award amount: 325,000 node-hours

Peer-Reviewed Publications

(Note: * = Equal Contribution)

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*, 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*, 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, 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*, 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), 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), 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, Orion Cohen, Ryan Kingsbury, Jason M. Munro, Rishabh Guha, Matthew K. Horton, and Kristin A. Persson. An open and accessible database for computational molecular chemistry. *In preparation*, 2023.

Evan Walter Clark Spotte-Smith, Samuel M. Blau, Daniel Barter, Noel J. Leon, Nikita S. Redkar, Chen Liao, and Kristin A. Persson. Chemical reaction networks explain gas evolution mechanisms in Mg-ion batteries. *ChemRxiv*, 2023. DOI:10.26434/chemrxiv-2023-tntkg.

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. *ChemRxiv*, 2023. DOI:10.26434/chemrxiv-2023-c8h70.

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, 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

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

Leadership & Service

2022 – **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
- **Current Role:** Graduate Student Representative

2022 – **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
- Review campus and UC system policies as they relate to LGBTQ+ campus members
- **Current Role:** Graduate Student Representative

2022 – **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
- **Current Role:** Materials Science and Engineering Delegate

2020 – **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
- **Current Role:** Vice-President
- **Previous Roles:** 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
- **Current Role:** 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