

# Evan Spotte-Smith

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

1066 56th St. Apt. B  
Oakland, CA 94608  
☎ 443-883-6957  
✉ ewcspottesmith@lbl.gov  
in evan-spotte-smith  
📧 espottesmith  
ORCID: 0000-0003-1554-197X  
Web: espottesmith.github.io

## 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
- 2020 – Present **Aniruddh Khanwale**.  
**Project:** Calculation of charge transfer rates through battery interphases
- 2021 – 2022 **Thea Petrocelli**, Intern, DOE Community College Internship (CCI) program.  
**Project:** Understanding salt decomposition in batteries from first principles
- 2021 – 2022 **Nikita Redkar**.  
**Project:** Learning electrochemical reaction products using natural language processing
- 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)

**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*, 2022.

**Evan Walter Clark Spotte-Smith\***, Alexander Epstein\*, Maxwell Venetos\*, Oxana Andriuc, and Kristin A. Persson. Assessing the accuracy of density functional approximations for predicting hydrolysis reaction kinetics. *In preparation*, 2022.

**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. *In review*, 2022. DOI:10.26434/chemrxiv-2022-4bd1p.

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. *In review*, 2022.

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. *In review*, 2022. DOI:10.26434/chemrxiv-2022-9557z.

**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. *In review*, 2022. DOI: 10.26434/chemrxiv-2021-c2gp3-v3.

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**. Leveraging big data and chemical reaction networks to explore and explain electrochemistry. ChemE Future Faculty Seminar Series (**Invited Talk**), 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**, Ronald L. Kam, Daniel Barter, Xiaowei Xie, Julian Self, Tingzheng Hou, Shyam Dwaraknath, Samuel M. Blau, and Kristin A. Persson. Using dynamic models to understand reactive competition in lithium-ion battery solid-electrolyte interphase formation. Accepted to 2021 AIChE Annual Meeting (withdrawn), 2021.

**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 – **Chancellor’s Advisory Committee on the LGBTQ+ Communities at Cal.**

- Present
- 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.**

- Present
- Advocate on behalf of materials science graduate students
  - Develop policies and legislation to promote the well-being of UC Berkeley graduate students
  - **Current Role:** Delegate

2020 – **UC Berkeley Materials Science and Engineering Graduate Student Council.**

- Present
- 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