

Evan Spotte-Smith

Evan Walter Clark Spotte-Smith
Computational Electrochemist

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Education

- 2019–2024 **Master of Science/Doctor of Philosophy**, *University of California, Berkeley (UC Berkeley)*.
Materials Science and Engineering Program
Advisor: Professor Kristin Persson
- 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)*.
 - Identify mechanistic origins of solid electrolyte interphase (SEI) formation in Li-ion and Mg-ion batteries.
 - Explore chemical reaction networks based on high-throughput density functional theory (DFT).
 - Analyze reactive competition in battery electrolytes through kinetic Monte Carlo (kMC) simulations.
 - Develop machine learning (ML) models to predict electrochemical reactivity
- 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 a reaction leading to exceptional heat capacity enhancement in aqueous thermal fluids.
- 2016 – 2019 **Lead Undergraduate Researcher, Herman Group**, *Columbia University*.
 - Studied nanoparticle self-assembly at liquid-liquid and liquid-air interfaces using time-resolved and space-resolved *in situ* synchrotron small angle x-ray scattering (SAXS).
 - Developed a novel cell architecture to improve SAXS signal.
 - Revealed an unexpected dominant mechanism driving self-assembly kinetics.

Teaching

- 2022 **Graduate Student Instructor**, *UC Berkeley Department of Chemistry*.
General Chemistry and Quantitative Analysis
- 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

- 2021 – Present **Thea Petrocelli**, Intern, Department of Energy Community College Internship (CCI) program.
Project: Comparing ion-assisted solvent decomposition pathways in multivalent-ion batteries
- 2021 – Present **Nikita Redkar**.
Project: Learning electrochemical reaction products using natural language processing
- 2020 – Present **Aniruddh Khanwale**.
Project: Exploring carbene reactivity in lithium-ion battery electrolytes
- 2020 – 2021 **Ronald Kam**.
Project: Kinetic modeling of lithium-ion solid-electrolyte interphase formation
Current Position: Graduate Student Research Assistant, Ceder Group, UC Berkeley

Honors & Awards

- 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 **Member**, 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.

Publications

(Note: * = Equal Contribution)

Evan Walter Clark Spotte-Smith*, Samuel M. Blau*, and Kristin A. Persson. First-principles dataset of molecules relevant to magnesium-ion battery solid electrolyte interphase formation. In preparation, 2022.

Thea B. Petrocelli, **Evan Walter Clark Spotte-Smith**, Alexander Epstein, and Kristin A. Persson. A comparative study of catalytic ion-assisted solvent decomposition in multivalent-ion batteries. In preparation, 2022.

Evan Walter Clark Spotte-Smith, Aniruddh Khanwale, Daniel Barter, Samuel M. Blau, and Kristin A. Persson. Carbene chemistry in the lithium-ion battery solid electrolyte interphase. In preparation, 2022.

Evan Walter Clark Spotte-Smith*, Ronald Kam*, Daniel Barter, Julian Self, Xiaowei Xie, Tingzheng Hou, Shyam Dwaraknath, Samuel M. Blau, and Kristin A. Persson. Towards a mechanistic model of solid-electrolyte interphase formation in lithium-ion batteries. In preparation, 2022.

Daniel Barter*, **Evan Walter Clark Spotte-Smith***, Nikita S. Redkar, Shyam Dwaraknath, Kristin A. Persson, and Samuel M. Blau. Predictive stochastic analysis of massive filter-based electrochemical reaction networks. *ChemRxiv*, 2022. DOI: 10.26434/chemrxiv-2021-c2gp3-v2.

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.

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.

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.

Posters & Presentations

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. Accepted to 2022 Gordon Research Conference in Electrochemistry, 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.

Leadership & Service

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| 2020 – Present | UC Berkeley Materials Science and Engineering Graduate Student Council. <ul style="list-style-type: none">Advocate to department administration and faculty for issues of importance to graduate studentsOrganize events to build community among materials science graduate studentsCoordinate anti-racist reading groups in collaboration with UC Berkeley Chemical Engineering departmentCurrent Role: Vice-PresidentPrevious Roles: Social Chair |
| 2020 – Present | CalACS College Application and Professional Support (CAPS). <ul style="list-style-type: none">Participate in weekly workshops with high school students to improve professional skillsDevelop long-term mentoring relationships with low-income, first-generation college applicantsProvide one-on-one assistance for college and job applicationsCurrent Role: Mentor |
| 2021 | Faculty Search Committee , UC Berkeley Department of Materials Science and Engineering. <ul style="list-style-type: none">Succeeded in hiring Xiaoyu (Rayne) Zheng for the position of Assistant Professor |
| 2020 – 2020 | Interstitials Mentorship Program. <ul style="list-style-type: none">Led peer-to-peer mentorship program for materials science communityPrevious Roles: Co-Director |
| 2020 | Faculty Search Committee , UC Berkeley Department of Materials Science and Engineering. <ul style="list-style-type: none">No candidate hired due to hiring freeze brought on by COVID-19 pandemic. |
| 2015 – 2018 | Columbia University Engineers Without Borders (CU-EWB). <ul style="list-style-type: none">Designed and implemented solar micro-grids for rural communities in the Teso Sub-Region of UgandaPrevious Roles: Engineering Mentor, President, Program Manager, Director of Grants, Program Liaison, Director of Operations |
| 2016 – 2018 | Columbia Educational Simulations (CESIMS). <ul style="list-style-type: none">Trained 25 student delegates at The Brooklyn Latin School for local and regional debate conferencesLed lessons and simulations on public speaking, history, and international affairsMentored students in order to prepare them for college and careersPrevious Roles: Academic Advisor |