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, Xiaowei Xie, Tingzheng Hou, Shyam Dwaraknath, Samuel M. Blau, and Kristin A. Persson. Towards a mechanistic model of solid-electrolyte interphase formation and evolution in lithium-ion batteries. *ChemRxiv*, 2022. DOI: 10.26434/chemrxiv-2022-n236n.

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

2020 – Present **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 Chemical Engineering department
- **Current Role**: Vice-President
- **Previous Roles**: Social Chair

2020 – Present **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

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

2020 **Faculty Search Committee**, UC Berkeley Department of Materials Science and Engineering.
- No candidate hired due to hiring freeze brought on by COVID-19 pandemic.

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