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

Aug. 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. Construct chemical reaction networks based on high-throughput density functional theory (DFT) to reveal optimal reaction pathways. Observe reactive competition through kinetic Monte Carlo (kMC) simulations.

June 2018 – Aug. 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 the highest specific heat capacity of any aqueous thermal fluid.

Sept. 2016– May 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 and revealed an unexpected dominant mechanism driving self-assembly kinetics.

Teaching

July 2020 **Instructor**, *Materials Project Workshop 2020*.
Pymatgen Foundations

Aug. 2018 – Dec. 2018 **Course Assistant**, *Columbia University Department of Applied Physics and Applied Mathematics*.
MSAE 3111: Thermodynamics, Kinetic Theory, and Statistical Mechanics

Mentorship

Mar. 2021 – Present **Nikita Redkar**, Research.
Project: Identifying plausible products of Mg-ion battery solid electrolyte interphase formation

Feb. 2020 – Present **Aniruddh Khanwale**, Research.
Project: Optimizing performance of computational reaction networks algorithms and data structures

June 2021 – Aug. 2021 **Thea Petrocelli**, Research, LBNL Community College Internship (CCI) program.
Project: Comparative Study of Solvent Decomposition Pathways for Multivalent-Ion Batteries

Jan. 2021 – May 2021 **Sahaj Singh Sidhu**, High School.

Mar. 2020 – Jan. 2021 **Ronald Kam**, Research.
Project: Kinetic modeling of lithium-ion solid-electrolyte interphase formation
Current Position: Graduate Student Research Assistant, Ceder Group, UC Berkeley

Sept. 2020 – Dec. 2020 **Kaitlan Nguyen**, High School.

Oct. 2019 – Jan. 2020 **Yuniba Yagües**, Graduate School.

Honors & Awards

2020 **Honorable Mention**, NSF Graduate Research Fellowship Program.

2019 **Honorable Mention**, NSF Graduate Research Fellowship Program.

2019 **Frank McQuiston Fellowship**, University of California, 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)

Samuel M. Blau*, Hetal D. Patel*, Daniel Barter, Aniruddh Khanwale, **Evan Walter Clark Spotte-Smith**, Ronald L. Kam, Mingjian Wen, Xiaowei Xie, Shyam Dwaraknath, and Kristin A. Persson. Mr.net: A python library for construction and analysis of molecular reaction networks. In preparation, 2021.

Evan Walter Clark Spotte-Smith*, Ronald Kam*, Daniel Barter, Xiaowei Xie, Julian Self, 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. In preparation, 2021.

Xiaowei Xie, **Evan Walter Clark Spotte-Smith**, Hetal Patel, Samuel M. Blau, and Kristin A. Persson. Data-driven prediction of formation mechanisms of lithium ethylene monocarbonate with an automated reaction network. ChemRxiv, 2021.

Lorena Alzate-Vargas, Srikanth Allu, Samuel Blau, **Evan Walter Clark Spotte-Smith**, Kristin A. Persson, and Jean-Luc Fattebert. Insight into sei growth in li-ion batteries using molecular dynamics and accelerated chemical reactions. In review, 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. Accepted in *Scientific Data*, 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*, 12:4931–4939, 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*, 12:1858–1868, 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.

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*, 124:23949–23963, 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, 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

Sept. 2020–Present — **Mentor**, 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 students from underprivileged backgrounds
- Provide one-on-one assistance for college and job applications

Sept. 2020–Present — **Social Chair**, UC Berkeley Materials Science and Engineering Graduate Student Council.
- Organize events to build community among materials science graduate students
- Design social events to help integrate first-year students into department culture
- Coordinate anti-racist reading groups in collaboration with UC Berkeley Chemical Engineering department

Feb. 2021 — **Member**, Faculty Search Committee, UC Berkeley Department of Materials Science and Engineering.
- Succeeded in hiring candidate for the position of Assistant Professor

Sept. 2020–Dec. 2020 — **Co-Director**, Interstitials Mentorship Program.
- Lead peer-to-peer mentorship program for materials science community
- Organize and coordinate educational events for undergraduate students
- Initiate and maintain relationships between student mentors and mentees

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

Sept. 2015–Dec. 2018 — **Columbia University Engineers Without Borders (CU-EWB)**.
- Leadership Roles:
  - 2018: Program Manager, Uganda Branch
  - 2017: President, CU-EWB
  - 2017: Director of Grants Team & Travel Team Lead, Uganda Branch
  - 2016: Director of Special Operations Team & Program Liaison, Uganda Branch
- Lead weekly meetings to discuss group progress, technical and logistical plans, and organizational finances
- Manage a team of 40 students to design off-grid solar power systems for rural Ugandan communities
- Draft and oversee an annual budget of $\$20,000$ gained from grants and fund-raising

Mar. 2016–May 2018 — **Academic Advisor**, *Columbia Educational Simulations (CESIMS).*
- Train 25 student delegates at The Brooklyn Latin School for local and regional MUN conferences
- Lead lessons and simulations on debate, public speaking, and international affairs
- Mentor students in order to prepare them for college and careers

Language Skills

- **English**: Native speaker
- **Spanish**: Basic conversational speaking, proficient reading
- **German**: Beginner