Evan Spotte-Smith

(they/them)

Assistant Prof. of Chemical Engineering

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Education

2023 **Doctor of Philosophy (Ph.D.)**, *University of California — Berkeley (UC Berkeley)*,
Program: Materials Science and Engineering
Advisor: Prof. Kristin A. Persson
Thesis: "On the Exploration of Electrochemical Reaction Cascades"

2021 **Master of Science (M.S.)**, *UC Berkeley*,
Program: Materials Science and Engineering

2019 **Bachelor of Science (B.S.)**, *Columbia University*,
Program: Materials Science and Engineering
Minor: Sustainable Engineering

Research Experience

2025 – **(Incoming) Assistant Professor of Chemical Engineering**, *Carnegie Mellon University (CMU)*,
Start Date: August 1, 2025

2024 – 2025 **Carnegie Bosch Institute Fellow**, *CMU*,
Advisor: Prof. Rachel C. Kurchin

2024 **Carnegie Bosch Institute Fellow**, *CMU*,
Advisor: Prof. Gabriel dos Passos Gomes

2019 – 2023 **Graduate Student Researcher**, *Lawrence Berkeley National Laboratory (LBNL)*,
Advisor: Prof. Kristin A. Persson

2023 **Cell Modeling Intern**, *Tesla Motors*

2018 – 2019 **Undergraduate Student Researcher**, *LBNL*,
Advisor: Dr. Anubhav Jain, Dr. Ravi Prasher

2016 – 2019 **Lead Undergraduate Researcher**, *Columbia University*,
Advisor: Prof. Irving P. Herman

Teaching Experience

Fall 2025 **Instructor**, *CMU*, Numerical Methods and ML for Chemical Engineers

Fall 2024 **Guest Lecturer**, *CMU*, "Data Science in the Chemical Sciences"

Spring 2022 **Graduate Student Instructor**, *UC Berkeley*, General Chemistry & Quantitative Analysis
Evaluation: median 7.0/7.0; mean 6.5/7.0

2020 **Instructor**, *Materials Project Workshop*, "Pymatgen Foundations"

Fall 2018 **Teaching Assistant**, *Columbia University*, Thermodynamics, Kinetic Theory, and Statistical Mechanics

Mentoring

2025 – **Punna Amornvivat**,
Project: Methods for machine learning on chemical reaction network hypergraphs

2024 – **Andrew Timmins**,
Project: Accelerated simulations of solid-state nucleation and phase transformations

2025 **Vanshika Singh**,
Project: Simulations of electrode protection in metal-mediated ammonia synthesis

2024 – 2025 **Shreya Pagaria**,
Project: Unsupervised phase identification from molecular dynamics simulations

2022 – 2023 **Laura Zichi**,
Project: Developing tools to simulate reactivity at dynamic fluid-solid interfaces

2021 – 2022 **Thea Bee Petrocelli**,
Project: First-principles explanations of electrolyte reactivity in Li-ion batteries

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 – 2022 **Ronald Kam**,
Project: Kinetic modeling of Li-ion battery solid-electrolyte interphase formation

Resources & Funding

2024 – 2026 **Synthesis Advanced Research Challenge**, *Toyota Research Institute*,
Project: Direct Introduction of Competition and Kinetics to Materials Mechanism and Reaction Network Prediction
Award type: Funding
Role: PI
Total award amount: $500,000

2025 – 2026 **National Artificial Intelligence Research Resource (NAIRR) Pilot**,
Project: Leveraging Machine Learned Interatomic Potentials to Predict Materials Synthesis Routes
Award type: High-performance computing allocation
Role: PI
Total award amount: 17,500 GPU-hours; 380,000 CPU-hours

2024 – 2025 **Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS)**, *National Science Foundation*,
Project: Rational Design of Electrolytes for Ammonia Synthesis Using Machine-Learned Potentials
Award type: High-performance computing allocation
Role: PI
Total award amount: 750,000 ACCESS credits

2020 – 2024 **Schrödinger, Inc.**,
Award type: Partnership
Role: Initiated partnership, lead point of contact
Total award amount: In kind, valued at $5,517,000

2021 – 2024 **High-Performance Computing**, *National Renewable Energy Laboratory*,
Project: Integrated Modeling and Machine Learning of Solid-Electrolyte Interface Reactions of the Si Anode
Award type: High-performance computing allocation
Role: Contributor
Total award amount: 6,884,000 node-hours

2020 – 2023 **Energy Research Computing Allocations Process**, *National Energy Research Supercomputing Center*,
Award type: High-performance computing allocation
Role: Contributor
Total award amount: 325,000 node-hours

Honors & Awards

2025 **Outstanding Reviewer**, Institute of Physics

2024 **Carnegie Bosch Institute Fellowship**, CMU

2024 **President's Postdoctoral Fellowship**, CMU (declined)

2024 **Pre-Faculty Workshop**, NextProf Nexus

2023 **1st Prize**, Winton-Kavli Research Pitch Competition

2023 **1st Prize**, Innovation Expo, Berkeley Energy & Resource Collaborative Energy Summit

2023 **Battery Student Slam Winner**, 241st Electrochemical Society Meeting

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 & Engineering

2019 **Clarendon Fund Scholarship**, University of Oxford (declined)

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

Peer-Reviewed Publications

(1) Guha*, R. D.; Vargas*, S.; Spotte-Smith, E. W. C.; Epstein, A. R.; Venetos, M.; Kingsbury, R.; Wen, M.; Blau, S. M.; Persson, K. A. HEPOM: Using Graph Neural Networks for the Accelerated Predictions of Hydrolysis Free Energies in Different pH Conditions. *Journal of Chemical Information and Modeling* **2025**

(2) Zichi*, L.; Barter*, D.; Sivonxay*, E.; Spotte-Smith, E. W. C.; Srinivaas, M. R.; ; Chan, E.; Persson, K. A.; Blau, S. M. RNMC: Kinetic Monte Carlo Implementations for Complex Reaction Networks. *The Journal of Open Source Software* **2024**, *9* (104), 7244

(3) Soto, M.; Fink, K.; Zweifel, C.; Weddle, P. J.; Spotte-Smith, E. W. C.; Veith, G.; Persson, K. A.; Colclasure, A. M.; Villers, B. J. Tremolet de. Solubilities of Ethylene and Carbon Dioxide Gases in Lithium-Ion Battery Electrolyte. *Journal of Chemical & Engineering Data* **2024**, *69* (6), 2236–2243

(4) Leon, N. J.; Illic, S.; Xie, X.; Jeong, H.; Yang, Z.; Wang, B.; Spotte-Smith, E. W. C.; Stern, C.; Hahn, N.; Zavadil, K.; Cheng, L.; Persson, K.; Connell, J.; Liao, C. Design Principles and Routes for Calcium Alkoxyaluminate Electrolytes. *The Journal of Physical Chemistry Letters* **2024**, *15* (19), 5096–5102

(5) Vijay, S.; Venetos, M.; Spotte-Smith, E. W. C.; Kaplan, A.; Wen, M.; Persson, K. A. CoeffNet: Predicting Activation Barriers Through a Constrained, Equivariant and Chemically-Interpretable Graph Neural Network. *Chemical Science* **2024**, *15* (8), 2923–2936

(6) Spotte-Smith*, E. W. C.; Vijay*, S.; Petrocelli, T. B.; Rinkel, B. L. D.; McCloskey, B. D.; Persson, K. A. A Critical Analysis of Chemical and Electrochemical Oxidation Mechanisms in Li-Ion Batteries. *The Journal of Physical Chemistry Letters* **2024**, *15* (2), 391–400

(7) Guha*, R. D.; Vargas*, S.; Spotte-Smith, E. W. C.; Epstein, A. R.; Venetos, M.; Wen, M.; Kingsbury, R.; Blau, S. M.; Persson, K. A. HEPOM: A Predictive Framework for Accelerated Hydrolysis Energy Predictions of Organic Molecules. *NeurIPS AI4Mat* **2023**

(8) Spotte-Smith, E. W. C.; Cohen, O. A.; Blau, S. M.; Munro, J. M.; Yang, R.; Guha, R. D.; Patel, H. D.; Vijay, S.; Huck, P.; Kingsbury, R.; Horton, M. K.; Persson, K. A. A Database of

Molecular Properties Integrated in the Materials Project. *Digital Discovery* **2023**, *2* (6), 1862–1882

(9) Weddle, P. J.; Spotte-Smith, E. W. C.; Verma, A.; Patel, H. D.; Fink, K.; Villers, B. J. Tremolet de; Schulze, M. C.; Blau, S. M.; Smith, K. A.; Persson, K. A.; Colclasure, A. M. Continuum-Level Modeling of Li-Ion Battery SEI by Upscaling Atomistically Informed Reaction Mechanisms. *Electrochimica Acta* **2023**, *468* (143121)

(10) Spotte-Smith, E. W. C.; Blau, S. M.; Barter, D.; Leon, N. J.; Hahn, N. T.; Redkar, N. S.; Zavadil, K. R.; Liao, C.; Persson, K. A. Chemical Reaction Networks Explain Gas Evolution Mechanisms in Mg-Ion Batteries. *Journal of the American Chemical Society* **2023**, *145* (22), 12181–12192

(11) Spotte-Smith*, E. W. C.; Epstein*, A. R.; Venetos, M.; Andriuc, O.; Persson, K. A. Assessing the Accuracy of Density Functional Approximations for Predicting Hydrolysis Reaction Kinetics. *Journal of Chemical Theory and Computation* **2023**, *19* (11), 3159–3171

(12) Wen, M.; Spotte-Smith, E. W. C.; Blau, S. M.; McDermott, M. J.; Krishnapriyan, A.; Persson, K. A. Chemical Reaction Networks and Opportunities for Machine Learning. *Nature Computational Science* **2023**, *3*, 12–24

(13) Spotte-Smith*, E. W. C.; Petrocelli*, T. B.; Patel, H. D.; Blau, S. M.; Persson, K. A. Elementary Decomposition Mechanisms of Lithium Hexafluorophosphate in Battery Electrolytes and Interphases. *ACS Energy Letters* **2023**, *8* (1), 347–355

(14) Spotte-Smith*, E. W. C.; Barter*, D.; Redkar, N. S.; Khanwale, A.; Dwaraknath, S.; Persson, K. A.; Blau, S. M. Predictive Stochastic Analysis of Massive Filter-Based Electrochemical Reaction Networks. *Digital Discovery* **2023**, *2* (123), 123–137

(15) Xie, X.; Leon, N. J.; Small, D. W.; Spotte-Smith, E. W. C.; Liao, C.; Persson, K. A. 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**, *126* (49), 20773–20785

(16) Spotte-Smith*, E. W. C.; Kam*, R.; Barter, D.; Xie, X.; Hou, T.; Dwaraknath, S.; Blau, S. M.; Persson, K. A. Toward a Mechanistic Model of Solid-Electrolyte Interphase Formation and Evolution in Lithium-Ion Batteries. *ACS Energy Letters* **2022**, *7*, 1446–1453

(17) Alzate-Vargas, L.; Blau, S.; Spotte-Smith, E. W. C.; Allu, S.; Persson, K. A.; Fattebert, J.-L. Insight into SEI Growth in Li-Ion Batteries Using Molecular Dynamics and Accelerated Chemical Reactions. *Journal of Physical Chemistry C* **2021**, *125* (34), 18588–18596

(18) Xie, X.; Spotte-Smith, E. W. C.; Wen, M.; Patel, H. D.; Blau, S. M.; Persson, K. A. Data-Driven Prediction of Formation Mechanisms of Lithium Ethylene Monocarbonate with an Automated Reaction Network. *Journal of the American Chemical Society* **2021**, *143* (33), 13245–13258

(19) Spotte-Smith*, E. W. C.; Blau*, S. M.; Xie, X.; Patel, H. D.; Wen, M.; Wood, B.; Dwaraknath, S.; Persson, K. A. Quantum Chemical Calculations of Lithium-Ion Battery Electrolyte and Interphase Species. *Scientific Data* **2021**, *8* (203)

(20) Blau, S. M.; Patel, H.; Spotte-Smith, E. W. C.; Xie, X.; Dwaraknath, S.; Persson, K. A. A Chemically Consistent Graph Architecture for Massive Reaction Networks Applied to Solid-Electrolyte Interphase Formation. *Chemical Science* **2021**, *12* (13), 4931–4939

(21) Wen, M.; Blau, S. M.; Spotte-Smith, E. W. C.; Dwaraknath, S.; Persson, K. A. BonDNet: A Graph Neural Network for the Prediction of Bond Dissociation Energies for Charged Molecules. *Chemical Science* **2021**, *12* (5), 1858–1868

(22) Hu, J.; Spotte-Smith, E. W. C.; Pan, B.; Garcia, R.; Colosqui, C.; Herman, I. P. 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* **2020**, *124* (13), 23949–23963

(23) Spotte-Smith, E. W. C.; Yu, P.; Blau, S. M.; Jain, A.; Prasher, R. S. Aqueous Diels-Alder Reactions for Thermochemical Storage and Heat Transfer Fluids Identified Using Density Functional Theory. *Journal of Computational Chemistry* **2020**, *41* (24), 2137–2150

(24) Hu, J.; Spotte-Smith, E. W. C.; Pan, B.; Herman, I. P. Improved Small-Angle X-Ray Scattering of Nanoparticle Self-Assembly Using a Cell with a Flat Liquid Surface. *Journal of Nanoparticle Research* **2019**, *21* (4), 71

Other Publications

(25) Spotte-Smith, E. W. C. Considering the Ethics of Large Machine Learning Models in the Chemical Sciences. *ChemRxiv (in review)* **2025**

(26) Horton, M. K.; Huck, P.; Yang, R. X.; Munro, J. M.; Dwaraknath, S.; Ganose, A. M.; Kingsbury, R. S.; Wen, M.; Shen, J.-X.; Mathis, T. S.; Kaplan, A. D.; Berket, K.; Riebesell, J.; George, J.; Rosen, A. S.; Spotte-Smith, E. W. C.; McDermott, M. J.; Cohen, O. A.; Dunn, A.; Kuner, M.; Rignanese, G.-M.; Hautier, G.; Petretto, G.; Waroquiers, D.; Griffin, S. M.; Neaton, J. B.; Chrzan, D. C.; Asta, M.; Cholia, S.; Ceder, G.; Ong, S. P.; Jain, A.; Persson, K. A. The Materials Project: A Decade of Materials Discovery. *In review* **2025**

(27) Sivonxay, E.; Attia, L.; Spotte-Smith, E. W. C.; Sanchez-Lengeling, B.; Xia, X.; Barter, D.; Chan, E. M.; Blau, S. M. Enabling Inverse Design of Nanoparticle Photophysics via Deep Learning on Heterogeneous Graphs. *ChemRxiv (in review)* **2025**

(28) Blau*, S.; Spotte-Smith*, E. W. C.; Wood, B.; Dwaraknath, S.; Persson, K. Accurate, Automated Density Functional Theory for Complex Molecules Using on-the-Fly Error Correction. *ChemRxiv* **2020**

Presentations

(29) Spotte-Smith, E. W. C. Data-Driven Design of Reactive Technologies: Case Studies in Energy Storage. *ACS Spring Meeting* **2025**

(30) Spotte-Smith, E. W. C.; Timmins, A.; Kurchin, R. C. Mechanistic Insights into Electrolyte Decomposition during Electrochemical Ammonia Synthesis from Machine-Learning Interatomic Potentials. *ACS Spring Meeting* **2025**

(31) Spotte-Smith, E. W. C.; Timmins, A.; Kurchin, R. C. Towards Rational Design of Sustainable Technologies with Data-Enabled Reactive Simulations. *Symposium on Responsible and Sustainable AI* **2025**

(32) Spotte-Smith, E. W. C. Towards Data-Driven Analysis of Sustainable Electrochemical Reactions. *Bosch Research and Technology Center Seminar* **2025**

(33) Spotte-Smith, E. W. C. Chemical Reaction Network Machine Learning (CRN-ML): A Frontier for Reactivity Studies. *AIMED Workshop on Heterogeneous Catalysis* **2024**

(34) Spotte-Smith, E. W. C. Datasets to Drive Practical Chemical Data Science. *Gordon Research Conference in Computational Chemistry* **2024**

(35) Spotte-Smith, E. W. C.; Hegazy, K.; Avaylon, M.; Vargas, S.; Cohen, O. A.; Mahoney, M. W.; Perciano, T.; Persson, K. A.; Blau, S. M. Challenging Molecular Machine Learning with Datasets of Ions and Radicals. *Gordon Research Seminar in Computational Chemistry* **2024**

(36) Spotte-Smith, E. W. C. Using Networks to Obtain Mechanistic Understanding in Electrochemistry. *Materials Science and Engineering Rising Stars Colloquium Series* **2024**

(37) Spotte-Smith, E. W. C. Rational Design of Sustainable Chemical Solutions with Reaction Networks and Data Science. *AIChE Annual Meeting* **2023**

(38) Spotte-Smith, E. W. C.; Blau, S. M.; Barter, D.; Leon, N. J.; Hahn, N. T.; Redkar, N. S.; Zavadil, K. R.; Liao, C.; Persson, K. A. Explaining Gas Evolution Mechanisms in Mg-Ion Batteries with Chemical Reaction Networks. *AIChE Annual Meeting* **2023**

(39) Spotte-Smith, E. W. C.; Cohen, O.; Blau, S. M.; Munro, J. M.; Kingsbury, R.; Guha, R. D.; Patel, H. D.; Vijay, S.; Yang, R.; Huck, P.; Horton, M. K.; Persson, K. A. MPcules: An Open and Accessible Database of Molecular Properties in the Materials Project. *ACS Fall 2023 Meeting* **2023**

(40) Spotte-Smith, E. W. C.; Petrocelli, T. B.; Patel, H. D.; Blau, S. M.; Persson, K. A. Revealing the Decomposition Mechanisms of Lithium Hexafluorophosphate in Battery Electrolytes and Interphases by First-Principles Simulations. *ACS Spring 2023 Meeting* **2023**

(41) Spotte-Smith, E. W. C.; Barter, D.; Kam, R. L.; Liao, C.; Blau, S. M.; Persson, K. A. Explaining Battery Electrolyte Decomposition with Chemical Reaction Networks. *Berkeley Energy & Resources Collaborative Energy Summit* **2023**

(42) Spotte-Smith, E. W. C. Leveraging Quantum Chemistry and Reaction Networks to Explore Electrochemical Cascades. *Pitzer Center for Theoretical Chemistry Seminar Series* **2022**

(43) Spotte-Smith, E. W. C. Leveraging Big Data and Chemical Reaction Networks to Explore and Explain Electrochemistry. *ChemE Future Faculty Seminar Series* **2022**

(44) Spotte-Smith, E. W. C.; Kam, R. L.; Barter, D.; Self, J.; Xie, X.; Hou, T.; Dwaraknath, S.; Blau, S. M.; Persson, K. A. A General Mechanistic Model of Early Solid-Electrolyte Interphase Formation in Lithium-Ion Batteries. *Gordon Research Conference in Electrochemistry* **2022**

(45) Spotte-Smith, E. W. C.; Kam, R. L.; Barter, D.; Xie, X.; Hou, T.; Dwaraknath, S.; Blau, S. M.; Persson, K. A. Towards a Mechanistic Explanation for Solid Electrolyte Interphase Formation and Evolution in Lithium-Ion Batteries. *American Conference on Theoretical Chemistry* **2022**

(46) Spotte-Smith, E. W. C.; Kam, R. L.; Barter, D.; Xie, X.; Hou, T.; Dwaraknath, S.; Blau, S. M.; Persson, K. A. Towards a Mechanistic Explanation for Solid Electrolyte Interphase Formation and Evolution in Lithium-Ion Batteries. *21st International Meeting on Lithium Batteries* **2022**

(47) Spotte-Smith, E. W. C.; Kam, R. L.; Barter, D.; Self, J.; Xie, X.; Hou, T.; Dwaraknath, S.; Blau, S. M.; Persson, K. A. Towards a Mechanistic Explanation for Solid Electrolyte Interphase Formation in Lithium-Ion Batteries. *241st Electrochemical Society Meeting* **2022**

(48) Spotte-Smith, E. W. C.; Blau, S. M.; Persson, K. A. GPS for the SEI: Charting Electrochemical Mechanisms with Reaction Networks. *241st Electrochemical Society Meeting* **2022**

(49) Spotte-Smith, E. W. C.; Blau, S. M.; Xie, X.; Wood, B.; Patel, H.; Dwaraknath, S.; Persson, K. A. Automatic Generation of Computational Reaction Networks for Unbiased Exploration of Chemical Pathways. *MRS Spring/Fall Meeting & Exhibit* **2020**

(50) Spotte-Smith, E. W. C.; Blau, S. M.; Wood, B.; Dwaraknath, S.; Persson, K. A. A Robust Computational Framework for High-Throughput Density Functional Theory Calculations for Electrochemical Application. *PRiME (ECS, ECSJ, & KECS Joint Meeting)* **2020**

(51) Spotte-Smith, E. W. C.; Yu, P.; Jain, A.; Prasher, R. Identifying Diels-Alder Reactions for Aqueous Thermal Storage Using Density Functional Theory. *MRS Spring Meeting and Exhibit* **2019**

Peer Review Experience

2025 *The Journal of Physical Chemistry* (x2), *Journal of Materials Chemistry A*, *ACS Applied Energy Materials*, JuliaCon 2025, NAIRR Pilot (x6), European Research Council Synergy Grant

2024 *The Journal of Open Source Software* (x2), *Scientific Data*, *Digital Discovery*, *Journal of Physics D: Applied Physics*, *Journal of Chemical Theory and Computation*, *Journal of Chemical Information and Modeling*, *Chemical Science*

2023 *ACS Nano*, *Journal of Chemical Information and Modeling*, *npj Computational Materials*

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

Organized Symposia & Workshops

2025 **Chemical Reaction Networks, Retrosynthesis, and Reaction Prediction**, *ACS Fall Meeting*

2025 **Symposium on Responsible and Sustainable AI**, *Carnegie Bosch Institute*

2023 **Kavli Career Development Workshop**, *UC Berkeley*

Leadership & Service

2025 – **Topic Editor**, *The Journal of Open Source Software*

2025 – **Mentor**, *DisabledInSTEM Mentorship Program*

2022 – 2023 **Materials Science and Engineering Delegate**, *UC Berkeley Graduate Assembly*

2022 – 2023 **Vice-President**, *UC Berkeley Materials Science and Engineering Graduate Student Council*,
Other Roles: Social Chair

2022 – 2023 **Mentor**, *CalACS College Application and Professional Support*

2020, 2021 **Graduate Student Representative**, *Materials Science and Engineering Faculty Search Committee*

2020 **Co-Director**, *Interstitials Mentorship Program*

2016 – 2019 **Academic Advisor**, *Columbia Educational Simulations*

2015 – 2019 **President**, *Columbia University Engineers Without Borders (CU-EWB)*,
Other Roles: Engineering Mentor, President, Program Manager, Director of Grants, Program Liaison, Director of Operations