curriculum vitæ of
Rachel C. Kurchin
Assistant Research Professor · Carnegie Mellon University · Materials Science and Engineering
rkurchin.github.io · rkurchin@cmu.edu · google scholar · github

Education

2014 – 2019 **Ph.D.** Materials Science and Engineering (GPA: 4.6/5.0) — Massachusetts Institute of Technology
Thesis title: "Computational Frameworks to Enable Accelerated Development of Defect-Tolerant Photovoltaic Materials"

2013 – 2014 **MPhil** Materials Science & Metallurgy (research-based) — University of Cambridge

2009 – 2013 **BS** Physics (Intensive) (GPA 3.9/4.0, magna cum laude) — Yale University

Past Research Positions

2019 – 2022 **Postdoctoral Fellow**, Mechanical Engineering, advised by V. Viswanathan — Carnegie Mellon University

2014 – 2019 **PhD student**, Materials Science and Engineering — Massachusetts Institute of Technology
Advised by T. Buonassisi (Mechanical Engineering) (committee members V. Stevanović, B. Yildiz, J. Grossman)

2016 – 2018 **Visiting student**, Solar Energy Research Facility — National Renewable Energy Laboratory
Summer stays advised by V. Stevanović

2013 – 2014 **MPhil student**, Materials Science & Metallurgy — University of Cambridge
Supervised by S. Smoukov, advised by Dame A. Donald (Physics)

2012 – 2013 **Undergraduate researcher**, Physics (senior thesis) — Yale University
Advised by M. L. Lee (Electrical Engineering)

Summer 2012 **REU Student**, Renewable Energy MRSEC, advised by T. Furtak (Physics) — Colorado School of Mines

2012 **Undergraduate researcher**, Physics, advised by C. Osuji (Chemical Engineeing) — Yale University

Summer 2011 **Undergraduate researcher**, Earth and Planetary Sciences — Weizmann Insistute of Science
Advised by I. Koren

Summer 2008 **High school summer researcher**, Laboratory for Laser Energetics — University of Rochester
Advised by R. S. Craxton and M. Wittman

Teaching Experience, Preparation, and Recognition

2023 **Instructor** — Carnegie Mellon University
27-100: Engineering the Materials of the Future
27-210: Materials Engineering Essentials

Guest Lecturer — Carnegie Mellon University
27-537/27-737: Data Analytics for Materials Science

2022 **Guest Lecturer** — Carnegie Mellon University
27-100: Engineering the Materials of the Future

2021 **Guest Lecturer** — Carnegie Mellon University
24-643/27-700: Energy Storage Materials and Systems
12-216: Introduction to Research Skills in CEE

2020 – 2023 **Guest Lecturer** — Carnegie Mellon University
12-623/24-623: Molecular Simulation of Materials
24-786: Bayesian Machine Learning

Future Faculty Program Alum, Eberly Center for Teaching Excellence — Carnegie Mellon University

2019 **Graduate Student Teaching Award**, Mat. Sci. and Eng. — Massachusetts Institute of Technology
Graduate Student Teaching Award, School of Engineering — Massachusetts Institute of Technology

2018 **Teaching Assistant** Massachusetts Institute of Technology
3.23: Electronic, Optical, and Magnetic Properties of Materials

2011 – 2013 **Science and Quantitative Reasoning Tutor**, Dean's Office Yale University

Honors

2023 Best Oral Presentation, Symposium EN10 Materials Research Society Fall Meeting
PASC Early Career Travel Award ACM SIGHPC
2022 DCOMP Travel Award APS Division of Computational Physics
DMP Post-Doctoral Travel Award APS Division of Materials Physics
2020 MolSSI Software Fellowship Molecular Sciences Software Institute
Rising Star in Computational and Data Sciences Oden Institute at UT Austin
2019 MFI Postdoctoral Fellowship CMU Manufacturing Futures Institute
CCE Symposium Poster Prize MIT Center for Computational Engineering
2018 Materials Day Best Poster Award MIT Materials Research Laboratory
2017 Blue Waters Graduate Fellowship National Center for Supercomputing Applications
2016 Total Energy Fellowship MIT Energy Initiative
Second Place, De Florez Award Competition MIT Department of Mechanical Engineering
2014 GRFP Honorable Mention National Science Foundation
2013 Gates Cambridge Scholarship Cambridge Gates Trust
Howard L. Schulz Prize Yale Physics Department
2012 Mellon Grant Pierson College at Yale University
REMRSEC REU Technical Achievement Award Colorado School of Mines Renewable Energy MRSEC
2009 Robert C. Byrd Honors Scholarship US Department of Education
Intel STS Semifinalist Intel Science Talent Search

Research Software Development

2021 – present **Co-Developer**, AtomsBase GitHub link
Julia interface for representing atomic structures, currently being used by >10 other Julia packages

2020 – present **Lead Developer**, ElectrochemicalKinetics GitHub link
Julia package for modeling and fitting of electrochemical reaction rate models

2020 – present **Lead Developer**, Chemellia GitHub link
Machine learning ecosystem for atomistic systems in the Julia Language

2017 – present **Lead Developer**, Bayesim GitHub link
Python package for Bayesian parameter estimation from experimental data using high-throughput simulation

Publications

Authors who equally contributed to a publication are marked with a †.

21. M. Babar, Z. Zhu, **R. C. Kurchin**, E. Kaxiras, and V. Viswanathan. "Twisto-Electrochemical Activity Volcanoes in Trilayer Graphene" *J. Am. Chem. Soc.* (2024)
20. X. Wang, J. Musielewicz, R. Tran, S. K. Ethirajan, X. Fu, H. Mera, J. R. Kitchin, **R. C. Kurchin**, and Z. W. Ulissi. "Generalization of graph-based active learning relaxation strategies across materials" *Mach. learn.: sci. technol.* (2024)
19. **R. C. Kurchin**, "Using Bayesian parameter estimation to learn more from data without black boxes" *Nat. Rev. Phys.* (2024)
18. **R. C. Kurchin**, D. Gandhi, and V. Viswanathan. "Nonequilibrium Electrochemical Phase Maps: Beyond Butler-Volmer Kinetics" *J. Phys. Chem. Lett.* 14, 7802–7807 (2023)

17. E. Annevelink[†], **R. C. Kurchin**[†], et al. "AutoMat: Automated Materials Discovery for Electrochemical systems." *MRS Bulletin* 47, (2022)
16. A. Mistry, ..., **R. C. Kurchin**, et al. "A minimal information set to enable verifiable theoretical battery research." *ACS Energy Lett.* 6, 11, 3831–3835 (2021)
15. **R. C. Kurchin** and V. Viswanathan. "Marcus-Hush-Chidsey kinetics at electrode-electrolyte interfaces." *J. Chem. Phys.* 153, 134706 (2020)
14. **R. C. Kurchin** et al. "How much physics is in a current-voltage curve? Inferring defect properties from photovoltaic device measurements." *IEEE JPV* 10, 1532–1537 (2020)
13. **R. C. Kurchin**, G. Romano, T. Buonassisi. "Bayesim: a tool for adaptive grid model fitting with Bayesian inference." *Comp. Phys. Comm.* 239, 161-165 (2019)
12. **R. C. Kurchin**[†], P. Gorai[†], Tonio Buonassisi, Vladan Stevanović. "Structural and chemical features giving rise to defect tolerance of binary semiconductors." *Chem. Mater.* 30, 5583–5592 (2018)
11. J. Correa-Baena, L. Nienhaus, **R. C. Kurchin**, et al. "A-site cation in inorganic $A_3Sb_2I_9$ perovskite influences structural dimensionality, exciton binding energy, and solar cell performance." *Chem. Mater.* 30, 3734–3742 (2018)
10. S. S. Shin, J. Correa-Baena, **R. C. Kurchin**, et al. "Solvent-engineering method to deposit compact bismuth-based thin films: mechanism and application to photovoltaics." *Chem. Mater.* 30, 336–343 (2017)
9. R. E. Brandt, **R. C. Kurchin**, et al. "Rapid semiconductor device characterization through Bayesian parameter estimation." *Joule* 1, 843–856 (2017)
8. R. Hoye, L. C. Lee, **R. C. Kurchin**, et al. "Strongly enhanced photovoltaic performance and defect physics of air-stable bismuth oxyiodide (BiOI)" *Adv. Mater.* 29, 1702176 (2017)
7. R. E. Brandt, J. R. Poindexter, P. Gorai, **R. C. Kurchin**, et al. "Searching for "defect-tolerant" photovoltaic materials: combined theoretical and experimental screening." *Chem. Mater.* 29, 4667–4674 (2017)
6. J. R. Poindexter, R. Hoye, L. Nienhaus, **R. C. Kurchin**, et al. "High tolerance to iron contamination in lead halide perovskite solar cells." *ACS Nano* 11, 7101–7109 (2017)
5. R. Hoye, ..., **R. C. Kurchin**, et al. "Perovskite-inspired photovoltaics: best practices in materials characterization and calculations." *Chem. Mater.* 29, 1964–1988 (2016)
4. D. B. Needleman, J. R. Poindexter, **R. C. Kurchin**, et al. "Economically sustainable scaling of photovoltaics to meet climate targets." *Energy Environ. Sci.* 9, 2122–2129 (2016)
3. A. Gufan, ..., **R. C. Kurchin**, et al. "Segmentation and tracking of marine cellular clouds observed by geostationary satellites." *Int. J. Remote Sens.* 37, 1055–1068 (2016)
2. R. Hoye, ..., **R. C. Kurchin**, et al. "Methylammonium bismuth iodide as a lead-free, stable hybrid organic-inorganic solar absorber." *Chem. Eur. J.* 22, 2605–2610 (2015)
1. R. E. Brandt, **R. C. Kurchin**, R. Hoye, et al. "Investigation of bismuth triiodide (BiI_3) for photovoltaic applications." *J. Phys. Chem. Lett.* 6, 4297–4302 (2015)

Presentations

Invited Talks

2024 *Materials Modeling: Bonding across Atoms, Code, and People* — Eindhoven, The Netherlands
JuliaCon **(keynote)**

Using Computation to Accelerate Materials Engineering, from the Atomistic to Device Scale — Seattle, WA
IEEE Photovoltaic Specialists Conference **(plenary)**

Learning from Data and Distributions to Accelerate Engineering of Energy Materials and Devices — Seattle, WA
MRS Spring Meeting

2023 *Materials Modeling (Data-Driven and Otherwise) in the Julia Language* — Virtual
Artificial Intelligence for Materials Science Workshop

It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box — Davos, Switzerland
Platform for Advanced Scientific Computing (PASC) Conference

It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box — Las Vegas, NV
American Physical Society March Meeting

Point Defects in Photovoltaics: From Materials to Devices — Evanston, IL
Snyder Group Meeting, Northwestern University

2022 *Science Stories with Julia* — Pittsburgh, PA (virtual)
Jordan Group Meeting, University of Pittsburgh

Building a Materials Computation Ecosystem in Julia — Ottawa, CA (virtual)
Institute of Data Science, Carleton University

Design of Defect-Tolerant Materials for Photovoltaic Applications — Chicago, IL
American Physical Society March Meeting

Building a Materials Computation Ecosystem in Julia — Cambridge, MA (virtual)
MIT CESMIX seminar

Accelerating Energy Materials Discovery with Computation — Boston, MA (virtual)
Boston University Materials Science seminar

2021 *Accelerating Energy Materials Discovery with Computation* — Atlanta, GA
Georgia Institute of Technology Department of Materials Science and Engineering

Do Me a Solid: Materials Modeling to Fight Climate Change — Pittsburgh, PA
Carnegie Mellon University Department of Civil and Environmental Engineering

2020 *High-Fidelity Accelerated Design of Electrochemical Systems* — online
Materials Science & Technology Conference

Graph Convolutional Networks for Atomic Structures — Cambridge, UK (virtual)
Cambridge Machine Learning Discussion Group

Marcus-Hush-Chidsey Kinetics at Solid Surfaces — online
Battery Modeling Webinar Series

Accelerating Energy Materials Discovery with Computation — Nuremberg, Germany (virtual)
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

Accelerating Energy Materials Discovery with Computation — Pittsburgh, PA (virtual)
Carnegie Mellon Department of Materials Science and Engineering

Accelerating Energy Materials Discovery with Computation — Urbana, IL
University of Illinois at Urbana-Champaign Department of Electrical & Computer Engineering

2019 *Bayesim Workshop* — Nuremberg, Germany (virtual)
Helmholtz Institute for Renewable Energy

2018 *Semiconductor Parameter Extraction (and more!) with Bayesian Inference* — Cambridge, MA
MIT Society of Industrial and Applied Mathematics

Contributed Talks

2023 *Modeling Electrochemical Reaction Rates at Fluid-Solid Interfaces* — Boston, MA
MRS Fall Meeting

Teaching Introductory Materials Science with Pluto Demos — Cambridge, MA
JuliaCon

2022 *Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation* — Chicago, IL
American Physical Society March Meeting

2021 *Introducing Chemellia: Machine Learning, with Atoms* — online
JuliaCon

Building a Chemistry and Materials Science Ecosystem in Julia — online
JuliaCon (Birds of a Feather discussion leader)

2018 *Computational Screening for Defect-Tolerant Semiconductors* — New London, NH
Gordon Research Seminar on Defects in Semiconductors

Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors — Sunriver, OR
Blue Waters Research Symposium

2017 *Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials* — Boston, MA
Materials Research Society Fall Meeting and Exhibit

2013 *Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications* — New Haven, CT
Yale Physics Department

2012 *Improving Active Layer Performance of Hybrid Photovoltaics by Nano Imprinting with Bulk Metallic Glass* — New Haven, CT
Yale Physics Department

Poster Presentations

2022 *Differentiable Modeling of Electrochemical Reaction Rates* — Ventura, CA
Gordon Research Seminar/Conference: Batteries

2020 *High-fidelity Accelerated Design of High-performance Electrochemical Systems* — online
NeurIPS Climate Change and AI Workshop

2019 *Measuring Real-World Quantities from Computer Simulation with Bayesian Inference* — Cambridge, MA
MIT de Florez Award Competition

Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods — Cambridge, MA
MIT CCE Symposium

2018 *Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods* — Cambridge, MA
MIT Materials Day

Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors — New London, NH
Gordon Research Seminar on Defects in Semiconductors

Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors — Sunriver, OR
Blue Waters Research Symposium

Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods — Waikoloa, HI
World Conference on Photovoltaic Energy Conversion

Design Principles for Defect-Tolerant Photovoltaic Absorbers — Cambridge, MA
MIT de Florez Award Competition

2016 *Quantitative Metrics for Defect Tolerance in Semiconductors* — Boston, MA
Materials Research Society Fall Meeting and Exhibit

Photovoltaics R&D: Thin Film Materials — Cambridge, MA
MIT Energy Night

Bayes-Sun Inference: Next-Generation Photovoltaics through Advanced Probabilistic Modeling — Cambridge, MA
MIT de Florez Award Competition

Statistical Inference of Materials Properties from Solar Cell Measurements — Cambridge, MA
Beyond 2016: MIT's Frontiers of the Future Symposium

2015 *Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbers* — Boston, MA
MRS Fall Meeting and Exhibit

Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials — Cambridge, MA
MIT Materials Day

Solar Energy Technology & Innovation in Mexico — Cambridge, MA
MIT Energy Initiative Solar Day

Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials — Golden, CO
NREL HOPE Workshop

2013 *Raman Spectroscopy of Silicon Quntum Dots* — Ithaca, NY
Northeast Conference for Undergraduate Women in Physics

2012 *Raman Spectroscopy of Silicon Quntum Dots* — Golden, CO
REMRSEC REU Poster Session

Service To The Scientific Community

Journal Editing

2021 – present Journal of Open-Source Software

Journal Reviewing

2023 – present Physical Review Letters
2022 – present Computer Physics Communications, APL Machine Learning
2021 – present Journal of Physical Chemistry, Chemistry of Materials, Journal of Physical Chemistry Letters, PR Materials, Computational Materials Science, IEEE Journal of Photovoltaics, Nature Computational Science
2020 – present NPJ Computational Materials
2019 – present Applied Energy Materials
2017 – present Energy & Environmental Science

Conference Service

2024 – present **Invited Organizer** — Electronic Materials Conference
2024 **Lead Organizer** — MolSSI workshop on Julia for Computational Molecular and Materials Science
May 2023 **Poster Session Judge** — CMU Meeting of the Minds
May 2023 **Technical Presentation Judge** — CMU MSE Graduate Symposium
2023 – 2024 **Poster Session Judge** — CMU Energy Week
March 2022 **Session Chair** — Scientific Machine Learning Webinar Series
March 2022 **Session Chair**, B67: Advanced Approaches in Modeling and Simulation of Defects — APS March Meeting
July 2021 **Session Chair, Volunteer** — JuliaCon
2021 – present **Reviewer** — JuliaCon
2019 – 2020 **Organizer** — Pittsburgh Conference for Undergraduate Women in Physics
2019 **Reviewer** — NeurIPS ML4PS Workshop
October 2019 **Poster Session Judge** — Pitt Science2019
2015 **Organizer** — Solar Energy Technology & Innovation in Mexico Workshop
January 2015 **Panelist** — Northeast Conference for Undergraduate Women in Physics
2011 – 2012 **Organizer** — Northeast Conference for Undergraduate Women in Physics

Leadership and University Service

2023 – present	**Member**, Undergraduate Education Committee	CMU MSE Department
2023 – present	**Member**, Open Science Advisory Board	CMU Libraries
October 2023	**Panelist, Mentor**	CMU MSE Rising Stars Workshop
April 2023	**Design Judge**, Buggy Design Competition	CMU Spring Carnival
2022 – present	**Working Group Chair**, Notebooks Now! Initiative	American Geophysical Union
2018 – 2019	**Member**, Graduate Student Advisory Group for Engineering	MIT School of Engineering
2018 – 2019	**Co-President**, Womxn of Materials Science	MIT DMSE
2017	**Mentor**, Solar Spring Break (service trip)	MIT Energy Initiative
2016 – 2019	**Member**, Energy Education Task Force	MIT Energy Initiative
2016 – 2019	**Member**, Solar Test Bed Steering Committee	MIT Office of Sustainability
2015 – 2017	**Co-Leader**, Solar/Grid Community	MIT Energy Club
2012 – 2013	**Co-Leader**, Project Bright	Yale Office of Sustainability
2012	**Co-President**, Society of Physics Students	Yale Physics Department

Outreach and Other Service

2022 – present	**Mentor**	Prison Mathematics Project
May 2022	**Guest Speaker**	Julia Gender Inclusive
2021 – present	**Volunteer**	Skype a Scientist
2021 – 2022	**Grand Award Judge**, Materials Science Division	Regeneron ISEF
Sumer 2021	**GSoC Mentor**, Julia Language (Chemellia)	Google Summer of Code
March 2014	**Demonstrator**	Cambridge Hands-On Science (CHaOS)

Other Skills and Activities

Foreign Languages

2003 – present **Spanish**, proficient
2010 – present **Hebrew**, intermediate
2020 – present **Mandarin**, beginner

Music: Violinist

2014 – 2019	Chamber Music Society, Gilbert & Sullivan Players, Musical Theater Guild	MIT
2009 – 2013	Jonathan Edwards College Philharmonic, pit orchestras for the Dramat, Gilbert & Sullivan Society, Opera Theatre of Yale College, and various independent productions	Yale

Athletics

2019 – 2021 **Finisher**, Ironman Maryland, Ironman 70.3 Musselman, and Pumpkinman Half Iron triathlons
2018 – 2019 **Treasurer**, MIT Triathlon Team
2014, 2018 **Finisher**, Stockholm and Marine Corps Marathons
2013 – 2014 **Rower**, Churchill College Boat Club (1st Women's VIII in May Bumps 2014)
2009 – 2012 **Member** (2009 – 2012), **Treasurer** (2010 – 2011), Yale Bulldog Cycling Team