curriculum vitæ of
Rachel C. Kurchin

Assistant Research Professor · Carnegie Mellon University · Materials Science and Engineering · (Physics by courtesy)

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, 2025 **Instructor** — Carnegie Mellon University
27-100: Engineering the Materials of the Future

2023 **Instructor** — Carnegie Mellon University
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 – present **Guest Lecturer** — Carnegie Mellon University
12-623/24-623: Molecular Simulation of Materials

2020 – 2023 **Guest Lecturer** — Carnegie Mellon University
24-786: Bayesian Machine Learning

2020 **Alum**, Future Faculty Program — Carnegie Mellon University
Eberly Center for Teaching Excellence

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** 3.23: Electronic, Optical, and Magnetic Properties of Materials	Massachusetts Institute of Technology
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 Julia interface for representing atomic structures, currently being used by >10 other Julia packages	GitHub link
2020 – 2022	**Lead Developer**, ElectrochemicalKinetics Julia package for modeling and fitting of electrochemical reaction rate models	GitHub link
2020 – 2022	**Lead Developer**, Chemellia Machine learning ecosystem for atomistic systems in the Julia Language	GitHub link
2017 – present	**Lead Developer**, Bayesim Python package for Bayesian parameter estimation from experimental data using high-throughput simulation	GitHub link

Publications

Advisees are underlined; authors who equally contributed to a publication are marked with a †.

24. P. Diehl, C. Soneson, **R. C. Kurchin**, R. C. Mounce, and D. S. Katz, "The Journal of Open Source Software (JOSS): Bringing Open-Source Software Practices to the Scholarly Publishing Community for Authors, Reviewers, Editors, and Publishers" *J. Lib. Schol. Comm.* (2025)

23. A. Timmins and **R. C. Kurchin**, "Addressing accuracy by prescribing precision: Bayesian error estimation of point defect energetics" *J. Appl. Phys.* (2024)

22. J. Tang, K. Jiang, P.-S. Tseng, **R. C. Kurchin**, L. M. Porter, and R. F. Davis. "Thermal stability and phase transformation of α-, $\kappa(\epsilon)$-, and γ-Ga_2O_3 films under different ambient conditions" *Appl. Phys. Lett.* (2024)

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)

Selected Invited Presentations

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
Materials Research Society Spring Meeting

2023 *Materials Modeling (Data-Driven and Otherwise) in the Julia Language* — Virtual
NIST 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

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 Department of Materials Science

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

Service To The Scientific Community

Journal Service

2021 – present **Editor** — Journal of Open Source Software

2020 – present **Reviewer**

Phys. Rev. Lett. (1), Comp. Phys. Comm. (1), PRX Energy (1), APL Mach. Learn. (1), J. Phys. Chem. (1), Chem. Mater. (1), J. Phys. Chem. Lett. (1), Phys. Rev. Mater. (6), Comput. Mater. Sci. (1), IEEE J-PV (1), Nat. Comp. Sci. (1), Npj Comput. Mater. (1)

Conference Service: Organization

2024 – present **Co-chair**, Local Committee — JuliaCon Global

2024 – present **Invited Organizer** — Electronic Materials Conference

2024 **Lead Organizer** — MolSSI workshop on Julia for Computational Molecular and Materials Science

2019 – 2020 **Organizer** — Pittsburgh Conference for Undergraduate Women in Physics

2015 **Organizer** — Solar Energy Technology & Innovation in Mexico Workshop

2011 – 2012 **Treasurer, Organizer** — Northeast Conference for Undergraduate Women in Physics

Conference Service: Other

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 **Reviewer** — NeurIPS ML4PS Workshop

October 2019 **Poster Session Judge** — Pitt Science2019

January 2015 **Panelist** — 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

2023 – present **Design Judge**, Buggy Design Competition — CMU Spring Carnival

October 2023 **Panelist, Mentor** — CMU MSE Rising Stars Workshop

2022 – 2024 **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

2024 – present **Teacher** — Leonard Gelfand Center for Service Learning and Outreach at CMU

2024 – present **Teacher** — Osher Lifelong Learning Institute at CMU

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)