curriculum vitæ of
Rachel C. Kurchin
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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 †.

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

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