# Rachel C. Kurchin

Assistant Research Professor  $\cdot$  Carnegie Mellon University  $\cdot$  Materials Science and Engineering

**≈** rkurchin.github.io □ rkurchin@cmu.edu **≈** google scholar **?** github

# EDUCATION

2014 – 2019	<b>Ph.D.</b> Materials Science and Engineering (GPA: 4.6/5.0) Thesis title: "Computational Frameworks to Enable Accelerated Developm	MASSACHUSETTS INSTITUTE OF TECHNOLOGY ent 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. Viswa	nathan 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	<b>Visiting student</b> , Solar Energy Research Facility Summer stays advised by V. Stevanović		
2013 – 2014	MPhil student, Materials Science & Metallurgy Supervised by S. Smoukov, advised by Dame A. Donald (Physics)	University of Cambridge	
2012 – 2013	Undergraduate researcher, Physics (senior thesis) Advised by M. L. Lee (Electrical Engineering)	YALE UNIVERSITY	
Summer 2012	REU Student, Renewable Energy MRSEC, advised by T. Furtak (P	hysics) Colorado School of Mines	
2012	Undergraduate researcher, Physics, advised by C. Osuji (Chemical	Engineeing) YALE UNIVERSITY	
Summer 2011	<b>Undergraduate researcher</b> , Earth and Planetary Sciences Advised by I. Koren	Weizmann Insistute of Science	
Summer 2008	<b>High school summer researcher</b> , Laboratory for Laser Energetics Advised by R. S. Craxton and M. Wittman	University of Rochester	
	TEACHING EXPERIENCE, PREPARATION, AND RECOGNIT	ION	
2023	Instructor 27-100: Engineering the Materials of the Future 27-210: Materials Engineering Essentials	Carnegie Mellon University	
	Guest Lecturer 27-537/27-737: Data Analytics for Materials Science	Carnegie Mellon University	
2022	Guest Lecturer 27-100: Engineering the Materials of the Future	Carnegie Mellon University	
2021	Guest Lecturer 24-643/27-700: Energy Storage Materials and Systems 12-216: Introduction to Research Skills in CEE	Carnegie Mellon University	
2020 – 2023	Guest Lecturer 12-623/24-623: Molecular Simulation of Materials 24-786: Bayesian Machine Learning	Carnegie Mellon University	
	Future Faculty Program Alum, Eberly Center for Teaching Excelle	nce Carnegie Mellon University	
2019	Graduate Student Teaching Award, Mat. Sci. and Eng. Graduate Student Teaching Award, School of Engineering	Massachusetts Institute of Technology Massachusetts Institute of Technology	

2018	Teaching Assistant	Massachusetts Institute of Technology	
	3.23: Electronic, Optical, and Magnetic Properties of Mat	erials	
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, current	tly 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		
1	Machine learning ecosystem for atomistic systems in the Julia Language		
2017 – present	Lead Developer, Bayesim	Lead Developer, Bayesim GITHUB LINK	
, 1	Python package for Bayesian parameter estimation from		

#### **PUBLICATIONS**

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

- 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<sup>†</sup>, **R. C. Kurchin**<sup>†</sup>, 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 inter-faces." *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**<sup>†</sup>, P. Gorai<sup>†</sup>, Tonio Buonassisi, Vladan Stevanović. "Structural and chemical features giving rise to defect tolerance of binary semiconductors." *Chem. Mater.* 30, 5583–5592 (2018)
- J. Correa-Baena, L. Nienhaus, R. C. Kurchin, et al. "A-site cation in inorganic A<sub>3</sub>Sb<sub>2</sub>I<sub>9</sub> perovskite influences structural dimensionality, exciton binding energy, and solar cell performance." *Chem. Mater.* 30, 3734–3742 (2018)
- 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)
- 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<sub>3</sub>) for photovoltaic applications." *J. Phys. Chem. Lett.* 6, 4297–4302 (2015)

## Presentations

## Invited Talks

2024

2022

Learning from Data and Distributions to Accelerate Engineering of Energy Materials and Devices

SEATTLE, WA
MRS Spring Meeting

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

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

2021

2020

2018

2023

2021

Accelerating Energy Materials Discovery with Computation

BOSTON, MA (VIRTUAL)

Boston University Materials Science seminar

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

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

Semiconductor Parameter Extraction (and more!) with Bayesian Inference

Cambridge, MA

MIT Society of Industrial and Applied Mathematics

Contributed Talks

Modeling Electrochemical Reaction Rates at Fluid-Solid Interfaces

BOSTON, MA

MRS Fall Meeting

Teaching Introductory Materials Science with Pluto Demos

Cambridge, MA

JuliaCon

Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation

CHICAGO, IL

American Physical Society March Meeting

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

Rachel C. Kurchin Curriculum Vitæ Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials 2017 Boston, MA Materials Research Society Fall Meeting and Exhibit Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications New Haven, CT 2013 Yale Physics Department Improving Active Layer Performance of Hybrid Photovoltaics by Nano Imprinting with Bulk Metallic Glass New Haven, CT 2012 Yale Physics Department POSTER PRESENTATIONS Differentiable Modeling of Electrochemical Reaction Rates VENTURA, CA 2022 Gordon Research Seminar/Conference: Batteries High-fidelity Accelerated Design of High-performance Electrochemical Systems ONLINE 2020 NeurIPS Climate Change and AI Workshop Measuring Real-World Quantities from Computer Simulation with Bayesian Inference Cambridge, MA 2019 MIT de Florez Award Competition Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods CAMBRIDGE, MA MIT CCE Symposium Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods Cambridge, MA 2018 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 Quantitative Metrics for Defect Tolerance in Semiconductors BOSTON, MA 2016 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 Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbers 2015 BOSTON, MA MRS Fall Meeting and Exhibit

Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials

Solar Energy Technology & Innovation in Mexico

MIT Materials Day

MIT Energy Initiative Solar Day

Cambridge, MA

Cambridge, MA

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

Journal of Physical Chemistry, Chemistry of Materials, Journal of Physical Chemistry Letters, PR Materials,

<sup>2021</sup> – present 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 S	Symposium
March 2023	Poster Session Judge	CMU EN	ergy Week
March 2022	Session Chair	Scientific Machine Learning Webi	nar Series
March 2022	Session Chair, B67: Advanced Approaches in	Modeling and Simulation of Defects APS MARC	h 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 So	CIENCE2019
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 Guest Speaker Julia Gender Inclusive May 2022 Volunteer 2021 – present SKYPE A SCIENTIST Grand Award Judge, Materials Science Division REGENERON ISEF 2021 - 2022 GSoC Mentor, Julia Language (Chemellia) GOOGLE SUMMER OF CODE Sumer 2021 Demonstrator CAMBRIDGE HANDS-ON SCIENCE (CHAOS) March 2014

## 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

Jonathan Edwards College Philharmonic, pit orchestras for the Dramat, Gilbert & Sullivan Society,

2009 - 2013 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