# 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) 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. Viswar	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	NATIONAL RENEWABLE ENERGY LABORATORY		
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 (Physics)  COLORADO SCHOOL OF MINE			
2012	Undergraduate researcher, Physics, advised by C. Osuji (Chemical Engineeing)  YALE UNIV		Yale University	
Summer 2011	<b>Undergraduate researcher</b> , Earth and Planetary Sciences Advised by I. Koren	,	Weizmann Insistute of Science	
	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 24-786: Bayesian Machine Learning		Carnegie Mellon University	
2022	Guest Lecturer 27-100: Engineering the Materials of the Future 12-623/24-623: Molecular Simulation of Materials		Carnegie Mellon University	
2021	Guest Lecturer 12-623/24-623: Molecular Simulation of Materials 24-643/27-700: Energy Storage Materials and Systems 12-216: Introduction to Research Skills in CEE		CARNEGIE MELLON UNIVERSITY	
2020	Guest Lecturer 12-623/24-623: Molecular Simulation of Materials 24-786: Bayesian Machine Learning (2 lectures)		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		SETTS INSTITUTE OF TECHNOLOGY SETTS INSTITUTE OF TECHNOLOGY	
2018	Teaching Assistant 3.23: Electronic, Optical, and Magnetic Properties of Materials	Massachu	SETTS INSTITUTE OF TECHNOLOGY	
2011 – 2013	Science and Quantitative Reasoning Tutor, Dean's Office		Yale University	

## Honors

2023	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 – present	Developer, ElectrochemicalKinetics Julia package for modeling and fitting of electrochemical reaction rate models	GITHUB LINK
2020 – present	Lead Developer, Chemellia Machine learning ecosystem for atomistic systems in the Julia Language	GITHUB LINK

Python package for Bayesian parameter estimation from experimental data using high-throughput simulation

## **PUBLICATIONS**

Developer, Bayesim

2017 - 2019

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

- 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)

GITHUB LINK

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<sub>3</sub>) for photovoltaic applications." J. Phys. Chem. Lett. 6, 4297-4302 (2015)

## Presentations

### INVITED TALKS

2023

2022

2021

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 Platform for Advanced Scientific Computing (PASC) Conference

DAVOS, SWITZERLAND

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

LAS VEGAS, NV

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

EVANSTON, IL.

Science Stories with Julia

Jordan Group Meeting, University of Pittsburgh

Building a Materials Computation Ecosystem in Julia

Ottawa, CA (virtual)

PITTSBURGH, PA (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

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 2020 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 Bayesim Workshop NUREMBERG, GERMANY (VIRTUAL) 2019 Helmholtz Institute for Renewable Energy Semiconductor Parameter Extraction (and more!) with Bayesian Inference CAMBRIDGE, MA 2018 MIT Society of Industrial and Applied Mathematics CONTRIBUTED TALKS Teaching Introductory Materials Science with Pluto Demos 2023 Cambridge, MA JuliaCon Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation CHICAGO, IL 2022 American Physical Society March Meeting Introducing Chemellia: Machine Learning, with Atoms ONLINE 2021 JuliaCon Building a Chemistry and Materials Science Ecosystem in Julia ONLINE JuliaCon (Birds of a Feather discussion leader) Computational Screening for Defect-Tolerant Semiconductors New London, NH 2018 Gordon Research Seminar on Defects in Semiconductors Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors SUNRIVER, OR Blue Waters Research Symposium Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials BOSTON, MA 2017 Materials Research Society Fall Meeting and Exhibit Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications New Haven, CT 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 Boston, MA 2015 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 Raman Spectroscopy of Silicon Quntum Dots ITHACA, NY 2013 Northeast Conference for Undergraduate Women in Physics Raman Spectroscopy of Silicon Quntum Dots GOLDEN, CO 2012 REMRSEC REU Poster Session SERVICE TO THE SCIENTIFIC COMMUNITY JOURNAL EDITING Journal of Open-Source Software 2021 – present JOURNAL REVIEWING 2022 – present Computer Physics Communications, APL Machine Learning Journal of Physical Chemistry, Chemistry of Materials, Journal of Physical Chemistry Letters, PR Materials, Computational Materials Science, IEEE Journal of Photovoltaics, Nature Computational Science 2021 - present 2020 – present NPJ Computational Materials Applied Energy Materials 2019 – present Energy & Environmental Science 2017 - present Conference Service Technical Presentation Judge CMU MSE GRADUATE SYMPOSIUM May 2023 Poster Session Judge CMU ENERGY WEEK March 2023

Session Chair SCIENTIFIC MACHINE LEARNING WEBINAR SERIES March 2022 Session Chair, B67: Advanced Approaches in Modeling and Simulation of Defects APS MARCH MEETING March 2022 Session Chair, Volunteer JULIACON July 2021 Reviewer 2021 – present JULIACON 2019 – 2020 Organizer PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS Reviewer NEURIPS ML4PS WORKSHOP 2019 Poster Session Judge PITT SCIENCE2019 October 2019 Organizer Solar Energy Technology & Innovation in Mexico Workshop Panelist NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS January 2015 Organizer NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS 2011 - 2012 Leadership/Outreach Design Judge CMU BUGGY DESIGN COMPETITION April 2023 2022 – present Working Group Chair NOTEBOOKS NOW! INITIATIVE PRISON MATHEMATICS PROJECT 2022 - present Mentor Guest Speaker Julia Gender Inclusive May 2022 Volunteer SKYPE A SCIENTIST 2021 - present Grand Award Judge, Materials Science Division REGENERON ISEF 2021 - 2022 GSoC Mentor, Julia Language (Chemellia) GOOGLE SUMMER OF CODE Sumer 2021 Member, Advisor-Advisee Relations Subcommittee 2018 – 2019 MIT GRAD STUDENT ADVISORY GROUP FOR ENGINEERING MIT Women of Materials Science Co-President 2018 – 2019 Mentor, Solar Spring Break (service trip) MIT Energy Initiative 2017 Member, Energy Education Task Force MIT Energy Initiative 2016 - 2019 Member, Solar Test Bed Steering Committee MIT OFFICE OF SUSTAINABILITY 2016 - 2019 2015 - 2017 Co-Leader, Solar/Grid Community MIT ENERGY CLUB Demonstrator CAMBRIDGE HANDS-ON SCIENCE (CHAOS) March 2014 Co-Leader, Project Bright YALE OFFICE OF SUSTAINABILITY 2012 - 2013 Yale Physics Department Co-President, Society of Physics Students OTHER SKILLS AND ACTIVITIES FOREIGN LANGUAGES Spanish, proficient 2003 – present Hebrew, intermediate 2010 – present Mandarin, beginner 2020 – present MUSIC: VIOLINIST Chamber Music Society, Gilbert & Sullivan Players, Musical Theater Guild MIT 2014 - 2019 Jonathan Edwards College Philharmonic, pit orchestras for the Dramat, Gilbert & Sullivan Society, Opera Theatre of Yale College, and various independent productions 2009 - 2013 YALE ATHLETICS Finisher, Ironman Maryland and Ironman 70.3 Musselman triathlons 2021 Finisher, Pumpkinman Half Iron Triathlon 2019 Treasurer, MIT Triathlon Team 2018 - 2019 Finisher, Stockholm and Marine Corps Marathons 2014, 2018 Rower, Churchill College Boat Club (1st Women's VIII in May Bumps 2014) 2013 - 2014

Member (2009 – 2012), Treasurer (2010 – 2011), Yale Bulldog Cycling Team

2009 - 2012