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

	EDCOMION .		
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. Viswan	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	Visiting student , 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 (Physics) COLORADO SCHOOL OF MI		
2012	Undergraduate researcher, Physics, advised by C. Osuji (Chemical Engineeing) YALE UNIVER		
Summer 2011	Undergraduate researcher , Earth and Planetary Sciences Advised by I. Koren	Weizmann Insistute of Science	
Summer 2008	High school summer researcher , 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 GITHUB LINK		
, 1	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 †.

- 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 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**[†], P. Gorai[†], 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 A₃Sb₂I₉ 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 (BiI₃) for photovoltaic applications." *J. Phys. Chem. Lett.* 6, 4297–4302 (2015)

Presentations

INVITED TALKS

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 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

PITTSBURGH, PA (VIRTUAL)

Jordan Group Meeting, University of Pittsburgh

Building a Materials Computation Ecosystem in Julia Institute of Data Science, Carleton University OTTAWA, CA (VIRTUAL)

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 2021 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 2019 NUREMBERG, GERMANY (VIRTUAL) 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 Modeling Electrochemical Reaction Rates at Fluid-Solid Interfaces 2023 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 2022 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) 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 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 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 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

Rachel C. Kurchin

Curriculum Vitæ

2013 Raman Spectroscopy of Silicon Quntum Dots

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

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,

²⁰²¹ – present Computational Materials Science, IEEE Journal of Photovoltaics, Nature Computational Science

Conference Service

May 2023 **Technical Presentation Judge** CMU MSE GRADUATE SYMPOSIUM

March 2023 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 – 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, 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

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

ITHACA, NY

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 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 Yale 2009 - 2013 ATHLETICS Finisher, Ironman Maryland, Ironman 70.3 Musselman, and Pumpkinman Half Iron triathlons 2019 – 2021 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)

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

2013 - 2014

2009 – 2012