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	Ph.D. Materials Science and Engineering (GPA: 4.6/5.0) Thesis title: "Computational Frameworks to Enable Accelerated Developm	MASSACHUSETTS INSTITUTE OF TECHNOLOGY nent 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 Venkat Viswanathan	Carnegie Mellon University	
2014 – 2019	PhD student, Materials Science and Engineering Advised by Tonio Buonassisi (Mechanical Engineering) (committee memb	MASSACHUSETTS INSTITUTE OF TECHNOLOGY vers V. Stevanović, B. Yildiz, J. Grossman)	
2016 – 2018	Visiting student , Solar Energy Research Facility Summer stays advised by Vladan Stevanović	National Renewable Energy Laboratory	
2013 – 2014	MPhil student, Materials Science & Metallurgy Supervised by Stoyan Smoukov, advised by Dame Athene Donald (Physics	University of Cambridge	
2012 – 2013	Undergraduate researcher, Physics (senior thesis) Advised by Minjoo Larry Lee (Electrical Engineering)	Yale University	
Summer 2012	REU Student, Renewable Energy MRSEC Advised by Thomas Furtak (Physics)	COLORADO SCHOOL OF MINES	
2012	Undergraduate researcher, Physics Advised by Chinedum Osuji (Chemical Engineeing)	Yale University	
Summer 2011	Undergraduate researcher , Earth and Planetary Sciences Advised by Ilan Koren	Weizmann Insistute of Science	
Summer 2008	High school summer researcher , Laboratory for Laser Energetics Advised by R. Stephen Craxton and Mark Wittman	University of Rochester	
	TEACHING EXPERIENCE, PREPARATION, AND RECOGNIT	ΓΙΟΝ	
2023	Instructor, 27-100: Engineering the Materials of the Future	Carnegie Mellon University	
2021	Guest Lecturer	Carnegie Mellon University	
	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		
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	ence 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 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

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 **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 – 2019 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 †.

- 17. E. Annevelink[†], **R. C. Kurchin**[†], et al. "AutoMat: Automated Materials Discovery for Electrochemical systems." *MRS Bulletin*, in press.
- 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)

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 (BiI₃) for photovoltaic applications." J. Phys. Chem. Lett. 6, 4297-4302 (2015)

202

202

I	Presentations	
I	nvited Talks	
	Science Stories with Julia ordan Group Meeting, University of Pittsburgh	Pittsburgh, PA (virtual)
	Building a Materials Computation Ecosystem in Julia nstitute of Data Science, Carleton University	Ottawa, CA (virtual)
	Design of Defect-Tolerant Materials for Photovoltaic Applications APS March Meeting	Chicago, IL
	Building a Materials Computation Ecosystem in Julia MIT CESMIX seminar	Cambridge, MA (virtual)
	Accelerating Energy Materials Discovery with Computation Boston University Materials Science seminar	Boston, MA (virtual)
	Accelerating Energy Materials Discovery with Computation Georgia Institute of Technology Department of Materials Science and Engineering	Atlanta, GA (virtual)
	Oo Me a Solid: Materials Modeling to Fight Climate Change Carnegie Mellon University Department of Civil and Environmental Engineering	Pittsburgh, PA
	High-Fidelity Accelerated Design of Electrochemical Systems Materials Science & Technology Conference	ONLINE
	Graph Convolutional Networks for Atomic Structures Cambridge Machine Learning Discussion Group	Cambridge, UK (virtual)
	Marcus-Hush-Chidsey Kinetics at Solid Surfaces Battery Modeling Webinar Series	ONLINE

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 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 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 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 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 Raman Spectroscopy of Silicon Quntum Dots 2013 ITHACA, NY Northeast Conference for Undergraduate Women in Physics 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 Computer Physics Communications 2022 - present 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 NPJ Computational Materials 2020 – present Applied Energy Materials 2019 – present Energy & Environmental Science 2017 – present Conference Service SCIENTIFIC MACHINE LEARNING WEBINAR SERIES Session Chair March 2022 Session Chair, B67: Advanced Approaches in Modeling and Simulation of Defects APS MARCH MEETING March 2022 Session Chair, Volunteer JULIACON July 2021

2021 – present

Reviewer

JULIACON

PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS
Reviewer

NeurIPS ML4PS Workshop

Organizer

Solar Energy Technology & Innovation in Mexico Workshop

Panelist

Northeast Conference for Undergraduate Women in Physics

Northeast Conference for Undergraduate Women in Physics

Northeast Conference for Undergraduate Women in Physics

LEADERSHIP/OUTREACH

May 2022 Guest Speaker Julia Gender Inclusive 2021 – present Volunteer SKYPE A SCIENTIST Grand Award Judge, Materials Science Division REGENERON ISEF 2021 – present GSoC Mentor, Julia Language (Chemellia) GOOGLE SUMMER OF CODE Sumer 2021 2018 – 2019 Member, Advisor-Advisee Relations Subcommittee MIT GRAD STUDENT ADVISORY GROUP FOR ENGINEERING Co-President MIT WOMEN OF MATERIALS SCIENCE 2018 - 2019 Mentor, Solar Spring Break (service trip) MIT Energy Initiative 2017 MIT ENERGY INITIATIVE Member, Energy Education Task Force 2016 – 2019 MIT OFFICE OF SUSTAINABILITY Member, Solar Test Bed Steering Committee 2016 – 2019 Co-Leader, Solar/Grid Community MIT ENERGY CLUB 2015 - 2017 Demonstrator CAMBRIDGE HANDS-ON SCIENCE (CHAOS) March 2014 Co-Leader, Project Bright YALE OFFICE OF SUSTAINABILITY 2012 - 2013 Co-President, Society of Physics Students Yale Physics Department 2012

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

Finisher, Ironman Maryland and Ironman 70.3 Musselman triathlons

Finisher, Pumpkinman Half Iron Triathlon

2018 – 2019 Treasurer, MIT Triathlon Team

Finisher, Stockholm and Marine Corps Marathons

Rower, Churchill College Boat Club (1st Women's VIII in May Bumps 2014)

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