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) 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 Advised by T. Buonassisi (Mechanical Engineering) (committee members V	nD student, Materials Science and Engineering Massachusetts Institute of Technology dvised 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	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 (P	hysics)	Colorado School of Mines		
2012	Undergraduate researcher, Physics, advised by C. Osuji (Chemical	Engineeing)	Yale University		
Summer 2011	Undergraduate researcher , Earth and Planetary Sciences Advised by I. Koren	,	Weizmann Insistute of Science		
	TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION				
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
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 †.

- 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)

11. 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)

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

EVANSTON, IL

Science Stories with Julia Jordan Group Meeting, University of Pittsburgh

Snyder Group Meeting, Northwestern University

PITTSBURGH, PA (VIRTUAL)

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

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 Cambridge, MA 2023 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 2018 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 Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials 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 2019 Cambridge, MA MIT de Florez Award Competition

	Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods MIT CCE Symposium	Cambridge, MA		
2018	Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods MIT Materials Day	Cambridge, MA		
	Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors Gordon Research Seminar on Defects in Semiconductors	New London, NH		
	Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors Blue Waters Research Symposium	Sunriver, OR		
	Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods World Conference on Photovoltaic Energy Conversion	Waikoloa, HI		
	Design Principles for Defect-Tolerant Photovoltaic Absorbers MIT de Florez Award Competition	Cambridge, MA		
2016	Quantitative Metrics for Defect Tolerance in Semiconductors Materials Research Society Fall Meeting and Exhibit	Boston, MA		
	Photovoltaics R&D: Thin Film Materials MIT Energy Night	Cambridge, MA		
	Bayes-Sun Inference: Next-Generation Photovoltaics through Advanced Probabilistic Modeling MIT de Florez Award Competition	Cambridge, MA		
	Statistical Inference of Materials Properties from Solar Cell Measurements Beyond 2016: MIT's Frontiers of the Future Symposium	Cambridge, MA		
2015	Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbance and Exhibit	orbers Boston, MA		
	Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials MIT Materials Day	Cambridge, MA		
	Solar Energy Technology & Innovation in Mexico MIT Energy Initiative Solar Day	Cambridge, MA		
	Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials NREL HOPE Workshop	Golden, CO		
2013	Raman Spectroscopy of Silicon Quntum Dots Northeast Conference for Undergraduate Women in Physics	Ithaca, NY		
2012	Raman Spectroscopy of Silicon Quntum Dots REMRSEC REU Poster Session	GOLDEN, CO		
	Service To The Scientific Community			
	Journal Editing			
2021 – present	Journal of Open-Source Software			
	Journal Reviewing			
2022 – present 2021 – 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			
2020 – present	NPJ Computational Materials			
2019 – present	Applied Energy Materials			
2017 – present	Energy & Environmental Science			

NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS

CONFERENCE SERVICE

Technical Presentation Judge CMU MSE GRADUATE SYMPOSIUM May 2023 March 2023 Poster Session Judge CMU ENERGY WEEK 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 July 2021 JULIACON 2021 – present Reviewer 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 2015 Panelist NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS January 2015

LEADERSHIP/OUTREACH

Organizer

2011 - 2012

Design Judge CMU BUGGY DESIGN COMPETITION April 2023 2022 – present Working Group Chair NOTEBOOKS NOW! INITIATIVE Mentor 2022 – present PRISON MATHEMATICS PROJECT Guest Speaker **JULIA GENDER INCLUSIVE** May 2022 2021 – present Volunteer SKYPE A SCIENTIST 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 MIT GRAD STUDENT ADVISORY GROUP FOR ENGINEERING 2018 – 2019 2018 – 2019 Co-President MIT Women of Materials Science 2017 Mentor, Solar Spring Break (service trip) MIT ENERGY INITIATIVE 2016 – 2019 Member, Energy Education Task Force MIT Energy Initiative Member, Solar Test Bed Steering Committee MIT OFFICE OF SUSTAINABILITY 2016 – 2019 Co-Leader, Solar/Grid Community MIT ENERGY CLUB 2015 - 2017 Demonstrator CAMBRIDGE HANDS-ON SCIENCE (CHAOS) March 2014 2012 - 2013 Co-Leader, Project Bright YALE OFFICE OF SUSTAINABILITY 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