Rachel C. Kurchin

 $Assistant \ Research \ Professor \cdot Carnegie \ Mellon \ University \cdot Materials \ Science \ and \ Engineering \cdot (Physics \ by \ Courtesy)$ $\ref{Research Professor} \cdot Carnegie \ Mellon \ University \cdot Materials \ Science \ and \ Engineering \cdot (Physics \ by \ Courtesy)$ $\ref{Research Professor} \cdot Carnegie \ Mellon \ University \cdot Materials \ Science \ and \ Engineering \cdot (Physics \ by \ Courtesy)$

	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. Viswanathan	Carnegie Mellon University	
2014 – 2019	PhD student, Materials Science and Engineering Massachusetts Institute of Technolog Advised by T. Buonassisi (Mechanical Engineering) (committee members V. Stevanović, B. Yildiz, J. Grossman)		
2016 – 2018	Visiting student, Solar Energy Research Facility NATION 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 MINES	
2012	Undergraduate researcher, Physics, advised by C. Osuji (Chemical Enginee	eing) Yale University	
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 RECOGNITION		
2023, 2025	Instructor 27-100: Engineering the Materials of the Future	Carnegie Mellon University	
2023	Instructor 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	Carnegie Mellon University	

12-623/24-623: Molecular Simulation of Materials

24-786: Bayesian Machine Learning

2020	Alum , Future Faculty Program Eberly Center for Teaching Excellence	Carnegie Mellon University	
2019	Graduate Student Teaching Award , Mat. Sci. and E Graduate Student Teaching Award , School of Engin	_	
2018	Teaching Assistant 3.23: Electronic, Optical, and Magnetic Properties of Mate	Massachusetts Institute of Technology 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 Julia interface for representing atomic structures, current	GITHUB LINK ly being used by >10 other Julia packages	
2020 - 2022	Lead Developer, ElectrochemicalKinetics GITHUB LINK Julia package for modeling and fitting of electrochemical reaction rate models		
2020 - 2022	Lead Developer, Chemellia Machine learning ecosystem for atomistic systems in the Julia Language		
2017 – present	Lead Developer, Bayesim	GitHub link	
/ Present	Python package for Bayesian parameter estimation from e		

PUBLICATIONS

Advisees are underlined; authors who equally contributed to a publication are marked with a †.

- 23. <u>A. Timmins</u> and **R. C. Kurchin**, "Addressing accuracy by prescribing precision: Bayesian error estimation of point defect energetics" *J. Appl. Phys.* (2024)
- 22. J. Tang, K. Jiang, P.-S. Tseng, R. C. Kurchin, L. M. Porter, and R. F. Davis. "Thermal stability and phase transformation of α -, $\kappa(\epsilon)$ -, and γ -Ga₂O₃ films under different ambient conditions" *Appl. Phys. Lett.* (2024)

21. M. Babar, Z. Zhu, R. C. Kurchin, E. Kaxiras, and V. Viswanathan. "Twisto-electrochemical activity volcanoes in trilayer graphene" J. Am. Chem. Soc. (2024)

- 20. X. Wang, J. Musielewicz, R. Tran, S. K. Ethirajan, X. Fu, H. Mera, J. R. Kitchin, R. C. Kurchin, and Z. W. Ulissi. "Generalization of graph-based active learning relaxation strategies across materials" *Mach. learn.: sci. technol.* (2024)
- R. C. Kurchin, "Using Bayesian parameter estimation to learn more from data without black boxes" Nat. Rev. Phys. (2024)
- 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)
- 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)
- R. C. Kurchin and V. Viswanathan. "Marcus-Hush-Chidsey kinetics at electrode-electrolyte interfaces."
 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)
- 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)
- I. 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

2024

2023

2021

2020

Materials Modeling: Bonding across Atoms, Code, and People

EINDHOVEN, THE NETHERLANDS

JuliaCon (keynote)

Using Computation to Accelerate Materials Engineering, from the Atomistic to Device Scale

Seattle, WA

IEEE Photovoltaic Specialists Conference (plenary)

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

2022 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

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

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

2019	Bayesim Workshop Helmholtz Institute for Renewable Energy	Nuremberg, Germany (virtual)
2018	Semiconductor Parameter Extraction (and more!) with Bayesian Inference MIT Society of Industrial and Applied Mathematics	Cambridge, MA
	Contributed Talks	
2023	Modeling Electrochemical Reaction Rates at Fluid-Solid Interfaces MRS Fall Meeting	Boston, MA
	Teaching Introductory Materials Science with Pluto Demos JuliaCon	Cambridge, MA
2022	Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation American Physical Society March Meeting	CHICAGO, IL
2021	Introducing Chemellia: Machine Learning, with Atoms JuliaCon	ONLINE
	Building a Chemistry and Materials Science Ecosystem in Julia JuliaCon (Birds of a Feather discussion leader)	ONLINE
2018	Computational Screening for Defect-Tolerant Semiconductors Gordon Research Seminar on Defects in Semiconductors	New London, NH
	Structural and Chemical Features Contributing to Defect Tolerance of Binary Semicon. Blue Waters Research Symposium	ductors Sunriver, OR
2017	Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials Research Society Fall Meeting and Exhibit	Materials Boston, MA
2013	Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Appli Yale Physics Department	cations New Haven, CT
2012	Improving Active Layer Performance of Hybrid Photovoltaics by Nano Imprinting with Bulk Metallic Glass Yale Physics Department	New Haven, CT
	Poster Presentations	
2022	Differentiable Modeling of Electrochemical Reaction Rates Gordon Research Seminar/Conference: Batteries	Ventura, CA
2020	High-fidelity Accelerated Design of High-performance Electrochemical Systems NeurIPS Climate Change and AI Workshop	ONLINE
2019	Measuring Real-World Quantities from Computer Simulation with Bayesian Inference MIT de Florez Award Competition	Cambridge, MA
	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 Semicon. Gordon Research Seminar on Defects in Semiconductors	ductors New London, NH
	Structural and Chemical Features Contributing to Defect Tolerance of Binary Semicon. Blue Waters Research Symposium	ductors Sunriver, OR

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 2013 ITHACA, NY 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 SERVICE** Editor 2021 – present JOURNAL OF OPEN SOURCE SOFTWARE 2020 – present Reviewer Phys. Rev. Lett. (1), Comp. Phys. Comm. (1), PRX Energy (1), APL Mach. Learn. (1), J. Phys. Chem. (1), Chem. Mater. (1), J.Phys. Chem. Lett. (1), Phys. Rev. Mater. (6), Comput. Mater. Sci. (1), IEEE J-PV (1), Nat. Comp. Sci. (1), Npj Comput. Mater. (1) CONFERENCE SERVICE: ORGANIZATION Co-chair, Local Committee JULIACON GLOBAL 2024 – present 2024 – present Invited Organizer ELECTRONIC MATERIALS CONFERENCE Lead Organizer MOLSSI WORKSHOP ON JULIA FOR COMPUTATIONAL MOLECULAR AND MATERIALS SCIENCE 2024 PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS Organizer 2019 - 2020 Organizer SOLAR ENERGY TECHNOLOGY & INNOVATION IN MEXICO WORKSHOP 2015 Treasurer, Organizer NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS 2011 - 2012 Conference Service: Other Poster Session Judge CMU MEETING OF THE MINDS

May 2023

May 2023 2023 - 2024 Technical Presentation Judge

Poster Session Judge

CMU MSE GRADUATE SYMPOSIUM

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 JULIACON July 2021 Reviewer 2021 – present JULIACON Reviewer NEURIPS ML4PS WORKSHOP 2019 Poster Session Judge PITT SCIENCE2019 October 2019 January 2015 Panelist NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS LEADERSHIP AND UNIVERSITY SERVICE 2023 – present Member, Undergraduate Education Committee CMU MSE DEPARTMENT Member, Open Science Advisory Board CMU LIBRARIES 2023 – present Design Judge, Buggy Design Competition CMU Spring Carnival 2023 – present Panelist, Mentor CMU MSE RISING STARS WORKSHOP October 2023 Working Group Chair, Notebooks Now! Initiative AMERICAN GEOPHYSICAL UNION 2022 - 2024 Member, Graduate Student Advisory Group for Engineering MIT SCHOOL OF ENGINEERING 2018 - 2019 2018 – 2019 Co-President, Womxn of Materials Science MIT DMSE 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 Co-Leader, Solar/Grid Community MIT ENERGY CLUB 2015 - 2017 2012 - 2013 Co-Leader, Project Bright YALE OFFICE OF SUSTAINABILITY Co-President, Society of Physics Students YALE PHYSICS DEPARTMENT 2012 OUTREACH AND OTHER SERVICE 2022 – present Mentor PRISON MATHEMATICS PROJECT 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 Demonstrator CAMBRIDGE HANDS-ON SCIENCE (CHAOS) March 2014 OTHER SKILLS AND ACTIVITIES FOREIGN LANGUAGES Spanish, proficient 2003 – present 2010 – present Hebrew, intermediate Mandarin, beginner 2020 – present MUSIC: VIOLINIST Chamber Music Society, Gilbert & Sullivan Players, Musical Theater Guild 2014 – 2019 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 Chattanooga Relay (cyclist) Finisher, Ironman Maryland 2021 Finisher, 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) 2013 - 2014 Member (2009 – 2012), Treasurer (2010 – 2011), Yale Bulldog Cycling Team 2009 - 2012