Rachel C. Kurchin

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

EDUCATION

2014 – 2019	Ph.D. Materials Science and Engineering (GPA: 4.6/5.0) MASSACHUSETTS INSTITUTE OF TECHNOLOG 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. Viswanath	an 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 NA Summer stays advised by V. Stevanović	tional 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 (Physi	cs) Colorado School of Mines					
2012	Undergraduate researcher, Physics, advised by C. Osuji (Chemical Engineeing) YALE UNIT						
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 – present	Guest Lecturer 12-623/24-623: Molecular Simulation of Materials	Carnegie Mellon University					
2020 - 2023	Guest Lecturer 24-786: Bayesian Machine Learning	Carnegie Mellon University					

2020	Alum, Future Faculty Program Eberly Center for Teaching Excellence	Carnegie Mellon University			
2019	Graduate Student Teaching Award, Mat. Sci. and E	ng. Massachusetts Institute of Technology			
	Graduate Student Teaching Award, School of Engin	_			
2018	Teaching Assistant 3.23: Electronic, Optical, and Magnetic Properties of Mate	Massachusetts Institute of Technology			
2011 – 2013	Science and Quantitative Reasoning Tutor, Dean's G	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 MIT Department of Mechanical Engineering			
	Second Place, De Florez Award Competition				
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	GITHUB LINK y being used by 310 other Julia packages			
2020 - 2022	Lead Developer , ElectrochemicalKinetics Julia package for modeling and fitting of electrochemical in	GITHUB LINK reaction rate models			
2020 - 2022	Lead Developer, Chemellia Machine learning ecosystem for atomistic systems in the Julia Language				
2017 – present	Lead Developer , Bayesim Python package for Bayesian parameter estimation from e	GITHUB LINK xperimental data using high-throughput simulation			
	Publications				

PUBLICATIONS

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

- 25. X. Wang, J. A. Loli, Z. W. Ulissi, M. P. de Boer, B. A. Webler, and R. C. Kurchin, "Constraint Active Search in Process Window Optimization for Powder Feed Directed Energy Deposition" *Integr. Mater. Manuf. Innov.* (2025)
- 24. P. Diehl, C. Soneson, **R. C. Kurchin**, R. C. Mounce, and D. S. Katz, "The Journal of Open Source Software (JOSS): Bringing Open-Source Software Practices to the Scholarly Publishing Community for Authors, Reviewers, Editors, and Publishers" *J. Lib. Schol. Comm.* (2025)

23. A. Timmins 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)
- 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)
- 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)
- 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)
- 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)
- 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

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2025

2024

2023

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2021

2020

Towards New Workflows in Computational Materials Science with Julia

FORT WORTH, TX

Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering

Materials Modeling: Bonding across Atoms, Code, and People JuliaCon (keynote)

EINDHOVEN, THE NETHERLANDS

Using Computation to Accelerate Materials Engineering, from the Atomistic to Device Scale IEEE Photovoltaic Specialists Conference (plenary)

Seattle, WA

Overview of Julia Ecosystems for Atomistic Modeling

Zurich, Switzerland

Platform for Advanced Scientific Computing (PASC) Conference

Learning from Data and Distributions to Accelerate Engineering of Energy Materials and Devices Materials Research Society Spring Meeting

SEATTLE, WA

Materials Modeling (Data-Driven and Otherwise) in the Julia Language

Virtual

NIST Artificial Intelligence for Materials Science Workshop

It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box

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

American Physical Society March Meeting

Las Vegas, NV

Evanston, IL

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

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 Department of Materials Science

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
Materials Science & Technology Conference

ONLINE

Mater

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 Materials Research Society Fall Meeting Teaching Introductory Materials Science with Pluto Demos Cambridge, MA JuliaCon Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation CHICAGO, IL 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 2017 Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials Boston, MA Materials Research Society Fall Meeting Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications 2013 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 2020 ONLINE NeurIPS Climate Change and AI Workshop

Rachel C. Kurchin Curriculum Vitæ 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 Quantum Dots ITHACA, NY 2013 Northeast Conference for Undergraduate Women in Physics Raman Spectroscopy of Silicon Quantum Dots GOLDEN, CO 2012 REMRSEC REU Poster Session SERVICE TO THE SCIENTIFIC COMMUNITY

JOURNAL SERVICE

2021 - present Editor (2021 - 2025), Associate Editor in Chief (2025 - present)

JOURNAL OF OPEN SOURCE SOFTWARE

2020 - present Reviewer

APL Mach. Learn. (1), Chem. Mater. (1), Comput. Mater. Sci. (1), Comp. Phys. Comm. (1), IEEE J-PV (1), J. Phys. Chem. (2), J. Phys. Chem. Lett. (1), Matter (1), Nat. Comp. Sci. (1), Npj Comput. Mater. (1), Phys. Rev. B (1), Phys. Rev. Lett. (1), Phys. Rev. Mater. (6), PRX Energy (1)

CONFERENCE SERVICE: ORGANIZATION

2024 - 2025 Co-chair, Local Committee JULIACON GLOBAL 2025 **Invited Organizer** ELECTRONIC MATERIALS CONFERENCE 2024 – present Lead Organizer MOLSSI WORKSHOP ON JULIA FOR COMPUTATIONAL MOLECULAR AND MATERIALS SCIENCE Organizer PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS 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 2023 - 2025 CMU MEETING OF THE MINDS Technical Presentation Judge CMU MSE GRADUATE SYMPOSIUM May 2023 Poster Session Judge 2023 - 2024 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 Reviewer NEURIPS ML4PS WORKSHOP 2019 Poster Session Judge PITT SCIENCE2019 October 2019 Panelist NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS January 2015

LEADERSHIP AND UNIVERSITY SERVICE

2025 – present Member, Community and Inclusion Committee CMU MSE DEPARTMENT Member, Undergraduate Education Committee CMU MSE DEPARTMENT 2023 – present 2023 – present Member, Open Science Advisory Board CMU LIBRARIES Design Judge, Buggy Design Competition 2023 - 2024 CMU Spring Carnival 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 MIT DMSE Co-President, Womxn of Materials Science 2018 – 2019 2017 Mentor, Solar Spring Break (service trip) MIT Energy Initiative Member, Energy Education Task Force 2016 - 2019 MIT Energy Initiative Member, Solar Test Bed Steering Committee MIT OFFICE OF SUSTAINABILITY 2016 – 2019 Co-Leader, Solar/Grid Community 2015 - 2017 MIT ENERGY CLUB Co-Leader, Project Bright YALE OFFICE OF SUSTAINABILITY 2012 - 2013 Co-President, Society of Physics Students Yale Physics Department 2012

OUTREACH AND OTHER SERVICE

2024 – present Teacher LEONARD GELFAND CENTER FOR SERVICE LEARNING AND OUTREACH AT CMU 2024 – present Teacher OSHER LIFELONG LEARNING INSTITUTE AT CMU 2022 – present Mentor PRISON MATHEMATICS PROJECT Guest Speaker Julia Gender Inclusive May 2022 Volunteer 2021 – present SKYPE A SCIENTIST Grand Award Judge, Materials Science Division 2021 - 2022 REGENERON ISEF 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 2020 – present Mandarin, beginner 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 Chattanooga Relay (cyclist) 2024 Finisher, Ironman Maryland 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