Rachel C. Kurchin

ASSISTANT RESEARCH PROFESSOR · CARNEGIE MELLON UNIVERSITY · MATERIALS SCIENCE AND ENGINEERING

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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 TECHNOLOGY
	Advised by T. Buonassisi (Mechanical Engineering) (committee members V. Stevanović, B. Yildiz, J. Grossman)	
2016 – 2018	**Visiting student**, Solar Energy Research Facility	NATIONAL RENEWABLE ENERGY LABORATORY
	Summer stays advised by V. Stevanović	
2013 – 2014	**MPhil student**, Materials Science & Metallurgy	UNIVERSITY OF CAMBRIDGE
	Supervised by S. Smoukov, advised by Dame A. Donald (Physics)	
2012 – 2013	**Undergraduate researcher**, Physics (senior thesis)	YALE UNIVERSITY
	Advised by M. L. Lee (Electrical Engineering)	
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 Engineeing)	YALE UNIVERSITY
Summer 2011	**Undergraduate researcher**, Earth and Planetary Sciences	WEIZMANN INSISTUTE OF SCIENCE
	Advised by I. Koren	
Summer 2008	**High school summer researcher**, Laboratory for Laser Energetics	UNIVERSITY OF ROCHESTER
	Advised by R. S. Craxton and M. Wittman	

TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION

2023	**Instructor**	CARNEGIE MELLON UNIVERSITY
	27-100: Engineering the Materials of the Future	
	27-210: Materials Engineering Essentials	
	Guest Lecturer	CARNEGIE MELLON UNIVERSITY
	27-537/27-737: Data Analytics for Materials Science	
2022	**Guest Lecturer**	CARNEGIE MELLON UNIVERSITY
	27-100: Engineering the Materials of the Future	
2021	**Guest Lecturer**	CARNEGIE MELLON UNIVERSITY
	24-643/27-700: Energy Storage Materials and Systems	
	12-216: Introduction to Research Skills in CEE	
2020 – 2023	**Guest Lecturer**	CARNEGIE MELLON UNIVERSITY
	12-623/24-623: Molecular Simulation of Materials	
	24-786: Bayesian Machine Learning	
	Future Faculty Program Alum, Eberly Center for Teaching Excellence	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**	Massachusetts Institute of Technology
	3.23: Electronic, Optical, and Magnetic Properties of Materials	
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, currently 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
	Machine learning ecosystem for atomistic systems in the Julia Language	
2017 – present	**Lead 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 †.

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)

19. **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)*

15. **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)*

11. J. Correa-Baena, L. Nienhaus, **R. C. Kurchin**, et al. "A-site cation in inorganic $A_3Sb_2I_9$ 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 (BiI_3) for photovoltaic applications." *J. Phys. Chem. Lett. 6, 4297–4302 (2015)*

Presentations

Invited Talks

| 2024 | *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 | |

2023	*Materials Modeling (Data-Driven and Otherwise) in the Julia Language* Artificial Intelligence for Materials Science Workshop	VIRTUAL
	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
2022	*Science Stories with Julia* Jordan Group Meeting, University of Pittsburgh	PITTSBURGH, PA (VIRTUAL)
	Building a Materials Computation Ecosystem in Julia Institute of Data Science, Carleton University	OTTAWA, CA (VIRTUAL)
	Design of Defect-Tolerant Materials for Photovoltaic Applications American Physical Society 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)
2021	*Accelerating Energy Materials Discovery with Computation* Georgia Institute of Technology Department of Materials Science and Engineering	ATLANTA, GA
	Do Me a Solid: Materials Modeling to Fight Climate Change Carnegie Mellon University Department of Civil and Environmental Engineering	PITTSBURGH, PA
2020	*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 Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)	NUREMBERG, GERMANY (VIRTUAL)
	Accelerating Energy Materials Discovery with Computation Carnegie Mellon Department of Materials Science and Engineering	PITTSBURGH, PA (VIRTUAL)
	Accelerating Energy Materials Discovery with Computation University of Illinois at Urbana-Champaign Department of Electrical & Computer Engineering	URBANA, IL
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 Semiconductors*
Blue Waters Research Symposium | SUNRIVER, OR |

| 2017 | *Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials*
Materials Research Society Fall Meeting and Exhibit | BOSTON, MA |

| 2013 | *Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications*
Yale Physics Department | 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 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   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

2015   *Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbers*   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

2013   *Raman Spectroscopy of Silicon Quntum Dots*   ITHACA, NY
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

2021 – present   Journal of Open-Source Software

JOURNAL REVIEWING

2023 – present   Physical Review Letters

2022 – present   Computer Physics Communications, APL Machine Learning

2021 – present   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

CONFERENCE SERVICE

May 2023	**Technical Presentation Judge**	CMU MSE GRADUATE SYMPOSIUM
2023 – 2024	**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	**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**, Undergraduate Education Committee	CMU MSE DEPARTMENT
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
2012	**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
2021 – present	**Volunteer**	Skype a Scientist
2021 – 2022	**Grand Award Judge**, Materials Science Division	Regeneron ISEF
Sumer 2021	**GSoC Mentor**, Julia Language (Chemellia)	Google Summer of Code
March 2014	**Demonstrator**	Cambridge Hands-On Science (CHAOS)

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 |
| 2009 – 2013 | Jonathan Edwards College Philharmonic, pit orchestras for the Dramat, Gilbert & Sullivan Society, Opera Theatre of Yale College, and various independent productions | Yale |

Athletics

2019 – 2021	**Finisher**, Ironman Maryland, Ironman 70.3 Musselman, and Pumpkinman Half Iron triathlons
2018 – 2019	**Treasurer**, MIT Triathlon Team
2014, 2018	**Finisher**, Stockholm and Marine Corps Marathons
2013 – 2014	**Rower**, Churchill College Boat Club (1st Women's VIII in May Bumps 2014)
2009 – 2012	**Member** (2009 – 2012), **Treasurer** (2010 – 2011), Yale Bulldog Cycling Team