Rachel C. Kurchin

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

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Thesis title: "Computational Frameworks to Enable Accelerated Development of Defect- 2013 - 2014 MPhil Materials Science & Metallurgy (research-based) BS Physics (Intensive) (GPA 3:9/4.0, magna cum laude) PAST RESEARCH POSITIONS 2019 - 2022 Postdoctoral Fellow, Mechanical Engineering, advised by V. Viswanathan PhD student, Materials Science and Engineering (committee members V. Stevanović, I 2016 - 2018 Visiting student, Solar Energy Research Facility NATIONAL R. Summer stays advised by V. Stevanović MPhil student, Materials Science & Metallurgy Supervised by S. Smoulkov, advised by Dame A. Donald (Physics) Undergraduate researcher, Physics (senior thesis) Advised by M. L. Lee (Electrical Engineering) Summer 2012 REU Student, Renewable Energy MRSEC, advised by T. Furtak (Physics) Undergraduate researcher, Physics, advised by C. Osuji (Chemical Engineering) Summer 2011 Undergraduate researcher, Earth and Planetary Sciences Advised by I. Koren Summer 2008 High school summer researcher, Laboratory for Laser Energetics Advised by R. S. Craston and M. Wittman TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION 10structor 27-100: Engineering the Materials of the Future 1022 Guest Lecturer 27-573/27-737: Data Analytics for Materials Science Guest Lecturer 27-100: Engineering the Materials of the Future 1022 Guest Lecturer 24-643/27-700: Energy Storage Materials and Systems 12-216: Introduction to Research Skills in CEE				
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24-643/27-700: Energy Storage Materials and Systems 12-216: Introduction to Research Skills in CEE	Carnegie Mellon University			
2020 2020 Cuest I return	Carnegie Mellon University			
2020 – 2023 Guest Lecturer 12-623/24-623: Molecular Simulation of Materials 24-786: Bayesian Machine Learning	Carnegie Mellon University			
Alum, Future Faculty Program Eberly Center for Teaching Excellence	Carnegie Mellon University			

2019	Graduate Student Teaching Award, Mat. Sci. and I	Eng. Massachusetts Institute of Technology	
	Graduate Student Teaching Award, School of Engin	neering Massachusetts Institute of Technology	
2018	Teaching Assistant	Massachusetts Institute of Technology	
	3.23: Electronic, Optical, and Magnetic Properties of Mate	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 1		
	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, current	ly being used by >10 other Julia packages	
2020 - 2022	Lead Developer , ElectrochemicalKinetics Julia package for modeling and fitting of electrochemical	GITHUB LINK reaction rate models	
2020 - 2022	Lead Developer, Chemellia	GitHub link	
	Machine learning ecosystem for atomistic systems in the J		
2017 – present	Lead Developer, Bayesim	GITHUB LINK	
	Python package for Bayesian parameter estimation from 6	experimental data using high-throughput simulation	

PUBLICATIONS

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

- 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)

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)
- 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)
- 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

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 2023 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 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 2021 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 2019 Bayesim Workshop NUREMBERG, GERMANY (VIRTUAL)

Helmholtz Institute for Renewable Energy

MIT Society of Industrial and Applied Mathematics

2018

Semiconductor Parameter Extraction (and more!) with Bayesian Inference

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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 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

Cambridge, MA Statistical Inference of Materials Properties from Solar Cell Measurements

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

2021 – present Editor JOURNAL OF OPEN SOURCE SOFTWARE

2020 – present Reviewer

2024

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

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 CMU MEETING OF THE MINDS May 2023

Technical Presentation Judge CMU MSE GRADUATE SYMPOSIUM May 2023

2023 - 2024 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 Reviewer NEURIPS ML4PS WORKSHOP Poster Session Judge PITT SCIENCE2019 October 2019 Panelist NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS January 2015 LEADERSHIP AND UNIVERSITY SERVICE Member, Undergraduate Education Committee CMU MSE DEPARTMENT 2023 – present Member, Open Science Advisory Board CMU LIBRARIES 2023 – present CMU Spring Carnival 2023 – present Design Judge, Buggy Design Competition October 2023 Panelist, Mentor CMU MSE RISING STARS WORKSHOP Working Group Chair, Notebooks Now! Initiative AMERICAN GEOPHYSICAL UNION 2022 - 2024 Member, Graduate Student Advisory Group for Engineering MIT SCHOOL OF ENGINEERING 2018 - 2019 Co-President, Womxn of Materials Science MIT DMSE 2018 - 2019 Mentor, Solar Spring Break (service trip) MIT Energy Initiative 2017 Member, Energy Education Task Force MIT ENERGY INITIATIVE 2016 – 2019 2016 – 2019 Member, Solar Test Bed Steering Committee MIT OFFICE OF SUSTAINABILITY Co-Leader, Solar/Grid Community MIT ENERGY CLUB 2015 - 2017 Co-Leader, Project Bright YALE OFFICE OF SUSTAINABILITY 2012 - 2013 Co-President, Society of Physics Students YALE PHYSICS DEPARTMENT OUTREACH AND OTHER SERVICE Teacher LEONARD GELFAND CENTER FOR SERVICE LEARNING AND OUTREACH AT CMU 2024 - present Teacher 2024 – present OSHER LIFELONG LEARNING INSTITUTE AT CMU 2022 – present Mentor PRISON MATHEMATICS PROJECT Guest Speaker May 2022 Julia Gender Inclusive 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 Demonstrator CAMBRIDGE HANDS-ON SCIENCE (CHAOS) March 2014 OTHER SKILLS AND ACTIVITIES FOREIGN LANGUAGES 2003 – present Spanish, proficient Hebrew, intermediate 2010 – present Mandarin, beginner 2020 – present 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 2019, 2021 Finisher, Ironman 70.3 Musselman and Pumpkinman Half Iron triathlons 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 2009 – 2012 Member (2009 – 2012), Treasurer (2010 – 2011), Yale Bulldog Cycling Team