Rachel C. Kurchin

$Assistant\ Research\ Professor\cdot Carnegie\ Mellon\ University\cdot Materials\ Science\ and\ Engineering$

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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 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 LABORA' Summer stays advised by V. Stevanović			
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 (Ph	nysics) 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		
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 RECOGNIT	ION		
2023	Instructor, 27-100: Engineering the Materials of the Future Guest Lecturer	Carnegie Mellon University		
	27-537/27-737: Data Analytics for Materials Science 24-786: Bayesian Machine Learning			
2022	Guest Lecturer	Carnegie Mellon University		
	27-100: Engineering the Materials of the Future 12-623/24-623: Molecular Simulation of Materials			
2021	Guest Lecturer	Carnegie Mellon University		
	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			
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 Exceller	nce 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		
2011 2072	3.23: Electronic, Optical, and Magnetic Properties of Materials Science and Overticative Resconing Tutor, Deep's Office	Virgiliamo		
2011 – 2013	Science and Quantitative Reasoning Tutor, Dean's Office	Yale University		

Honors

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 **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 – 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 †.

- 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)
- 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)
- 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)
- 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	
2023	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)

Accelerating Energy Materials Discovery with Computation

ATLANTA, GA (VIRTUAL)

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

Graph Convolutional Networks for Atomic Structures

CAMBRIDGE, UK (VIRTUAL)

Cambridge Machine Learning Discussion Group

Boston University Materials Science seminar

2021

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 MIT Society of Industrial and Applied Mathematics Contributed Talks Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation CHICAGO IL 2022 American Physical Society March Meeting Introducing Chemellia: Machine Learning, with Atoms 2021 ONLINE 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 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 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 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 Cambridge, MA and Bayesian Inference Methods 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 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 2013 Raman Spectroscopy of Silicon Quntum Dots 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 EDITING Journal of Open-Source Software 2021 – present JOURNAL REVIEWING APL Machine Learning 2022 – present Computer Physics Communications 2022 – 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 2021 – present NPJ Computational Materials 2020 – present 2019 – present Applied Energy Materials Energy & Environmental Science 2017 – present Conference Service 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 JULIACON 2021 – present PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS 2019 – 2020 Organizer 2019 Reviewer NEURIPS ML4PS WORKSHOP Organizer SOLAR ENERGY TECHNOLOGY & INNOVATION IN MEXICO WORKSHOP 2015 Panelist NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS January 2015 NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS Organizer 2011 - 2012 LEADERSHIP/OUTREACH 2022 – present Working Group Chair NOTEBOOKS NOW! INITIATIVE 2022 – present Mentor PRISON MATHEMATICS PROJECT Guest Speaker Julia Gender Inclusive May 2022 Volunteer 2021 – present SKYPE A SCIENTIST 2021 – present Grand Award Judge, Materials Science Division REGENERON ISEF GSoC Mentor, Julia Language (Chemellia) GOOGLE SUMMER OF CODE Sumer 2021 2018 – 2019 Member, Advisor-Advisee Relations Subcommittee MIT GRAD STUDENT ADVISORY GROUP FOR ENGINEERING Co-President MIT Women of Materials Science 2018 – 2019 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 2015 - 2017 Co-Leader, Solar/Grid Community MIT ENERGY CLUB Demonstrator CAMBRIDGE HANDS-ON SCIENCE (CHAOS) March 2014 Co-Leader, Project Bright 2012 - 2013 YALE OFFICE OF SUSTAINABILITY Co-President, Society of Physics Students YALE PHYSICS DEPARTMENT 2012 OTHER SKILLS AND ACTIVITIES FOREIGN LANGUAGES Spanish, proficient 2003 – present Hebrew, intermediate 2010 – present Mandarin, beginner 2020 – present 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 2021 Finisher, Pumpkinman Half Iron Triathlon 2019 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