

curriculum vitae of  
**Rachel C. Kurchin**

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

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## EDUCATION

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2014 – 2019	<b>Ph.D.</b> Materials Science and Engineering (GPA: 4.6/5.0) Thesis title: “Computational Frameworks to Enable Accelerated Development of Defect-Tolerant Photovoltaic Materials”	MASSACHUSETTS INSTITUTE OF TECHNOLOGY
2013 – 2014	<b>MPhil</b> Materials Science & Metallurgy (research-based)	UNIVERSITY OF CAMBRIDGE
2009 – 2013	<b>BS</b> Physics (Intensive) (GPA 3.9/4.0, magna cum laude)	YALE UNIVERSITY

## PAST RESEARCH POSITIONS

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2019 – 2022	<b>Postdoctoral Fellow</b> , Mechanical Engineering, advised by V. Viswanathan	CARNEGIE MELLON UNIVERSITY
2014 – 2019	<b>PhD student</b> , Materials Science and Engineering Advised by T. Buonassisi (Mechanical Engineering) (committee members V. Stevanović, B. Yildiz, J. Grossman)	MASSACHUSETTS INSTITUTE OF TECHNOLOGY
2016 – 2018	<b>Visiting student</b> , Solar Energy Research Facility Summer stays advised by V. Stevanović	NATIONAL RENEWABLE ENERGY LABORATORY
2013 – 2014	<b>MPhil student</b> , Materials Science & Metallurgy Supervised by S. Smoukov, advised by Dame A. Donald (Physics)	UNIVERSITY OF CAMBRIDGE
2012 – 2013	<b>Undergraduate researcher</b> , Physics (senior thesis) Advised by M. L. Lee (Electrical Engineering)	YALE UNIVERSITY
Summer 2012	<b>REU Student</b> , Renewable Energy MRSEC, advised by T. Furtak (Physics)	COLORADO SCHOOL OF MINES
2012	<b>Undergraduate researcher</b> , Physics, advised by C. Osuji (Chemical Engineering)	YALE UNIVERSITY
Summer 2011	<b>Undergraduate researcher</b> , Earth and Planetary Sciences Advised by I. Koren	WEIZMANN INSTITUTE OF SCIENCE
Summer 2008	<b>High school summer researcher</b> , Laboratory for Laser Energetics Advised by R. S. Craxton and M. Wittman	UNIVERSITY OF ROCHESTER

## TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION

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2023	<b>Instructor</b> 27-100: Engineering the Materials of the Future 27-210: Materials Engineering Essentials	CARNEGIE MELLON UNIVERSITY
	<b>Guest Lecturer</b> 27-537/27-737: Data Analytics for Materials Science	CARNEGIE MELLON UNIVERSITY
2022	<b>Guest Lecturer</b> 27-100: Engineering the Materials of the Future	CARNEGIE MELLON UNIVERSITY
2021	<b>Guest Lecturer</b> 24-643/27-700: Energy Storage Materials and Systems 12-216: Introduction to Research Skills in CEE	CARNEGIE MELLON UNIVERSITY
2020 – 2023	<b>Guest Lecturer</b> 12-623/24-623: Molecular Simulation of Materials 24-786: Bayesian Machine Learning	CARNEGIE MELLON UNIVERSITY
	<b>Future Faculty Program Alum</b> , Eberly Center for Teaching Excellence	CARNEGIE MELLON UNIVERSITY
2019	<b>Graduate Student Teaching Award</b> , Mat. Sci. and Eng.	MASSACHUSETTS INSTITUTE OF TECHNOLOGY
	<b>Graduate Student Teaching Award</b> , School of Engineering	MASSACHUSETTS INSTITUTE OF TECHNOLOGY

2018	<b>Teaching Assistant</b> 3.23: Electronic, Optical, and Magnetic Properties of Materials	MASSACHUSETTS INSTITUTE OF TECHNOLOGY
2011 – 2013	<b>Science and Quantitative Reasoning Tutor</b> , Dean's Office	YALE UNIVERSITY

## HONORS

2023	Best Oral Presentation, Symposium EN10 PASC Early Career Travel Award	MATERIALS RESEARCH SOCIETY FALL MEETING ACM SIGHPC
2022	DCOMP Travel Award DMP Post-Doctoral Travel Award	APS DIVISION OF COMPUTATIONAL PHYSICS APS DIVISION OF MATERIALS PHYSICS
2020	MolSSI Software Fellowship Rising Star in Computational and Data Sciences	MOLECULAR SCIENCES SOFTWARE INSTITUTE ODEN INSTITUTE AT UT AUSTIN
2019	MFI Postdoctoral Fellowship CCE Symposium Poster Prize	CMU MANUFACTURING FUTURES INSTITUTE 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 Second Place, De Florez Award Competition	MIT ENERGY INITIATIVE MIT DEPARTMENT OF MECHANICAL ENGINEERING
2014	GRFP Honorable Mention	NATIONAL SCIENCE FOUNDATION
2013	Gates Cambridge Scholarship Howard L. Schulz Prize	CAMBRIDGE GATES TRUST YALE PHYSICS DEPARTMENT
2012	Mellon Grant REMRSEC REU Technical Achievement Award	PIERSON COLLEGE AT YALE UNIVERSITY COLORADO SCHOOL OF MINES RENEWABLE ENERGY MRSEC
2009	Robert C. Byrd Honors Scholarship Intel STS Semifinalist	US DEPARTMENT OF EDUCATION INTEL SCIENCE TALENT SEARCH

## RESEARCH SOFTWARE DEVELOPMENT

2021 – present	<b>Co-Developer</b> , AtomsBase Julia interface for representing atomic structures, currently being used by >10 other Julia packages	<a href="#">GITHUB LINK</a>
2020 – present	<b>Lead Developer</b> , ElectrochemicalKinetics Julia package for modeling and fitting of electrochemical reaction rate models	<a href="#">GITHUB LINK</a>
2020 – present	<b>Lead Developer</b> , Chemellia Machine learning ecosystem for atomistic systems in the Julia Language	<a href="#">GITHUB LINK</a>
2017 – present	<b>Lead Developer</b> , Bayesim Python package for Bayesian parameter estimation from experimental data using high-throughput simulation	<a href="#">GITHUB LINK</a>

## PUBLICATIONS

Authors who equally contributed to a publication are marked with a †.

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<sup>†</sup>, **R. C. Kurchin**<sup>†</sup>, 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 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**<sup>†</sup>, P. Gorai<sup>†</sup>, 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<sub>3</sub>Sb<sub>2</sub>I<sub>9</sub> 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<sub>3</sub>) for photovoltaic applications." *J. Phys. Chem. Lett.* 6, 4297–4302 (2015)

## PRESENTATIONS

### INVITED TALKS

2024	<i>Learning from Data and Distributions to Accelerate Engineering of Energy Materials and Devices</i> MRS Spring Meeting	SEATTLE, WA
2023	<i>Materials Modeling (Data-Driven and Otherwise) in the Julia Language</i> Artificial Intelligence for Materials Science Workshop	VIRTUAL
	<i>It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box</i> Platform for Advanced Scientific Computing (PASC) Conference	DAVOS, SWITZERLAND
	<i>It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box</i> American Physical Society March Meeting	LAS VEGAS, NV
	<i>Point Defects in Photovoltaics: From Materials to Devices</i> Snyder Group Meeting, Northwestern University	EVANSTON, IL

2022	<i>Science Stories with Julia</i> Jordan Group Meeting, University of Pittsburgh	PITTSBURGH, PA (VIRTUAL)
	<i>Building a Materials Computation Ecosystem in Julia</i> Institute of Data Science, Carleton University	OTTAWA, CA (VIRTUAL)
	<i>Design of Defect-Tolerant Materials for Photovoltaic Applications</i> American Physical Society March Meeting	CHICAGO, IL
	<i>Building a Materials Computation Ecosystem in Julia</i> MIT CESMIX seminar	CAMBRIDGE, MA (VIRTUAL)
	<i>Accelerating Energy Materials Discovery with Computation</i> Boston University Materials Science seminar	BOSTON, MA (VIRTUAL)
2021	<i>Accelerating Energy Materials Discovery with Computation</i> Georgia Institute of Technology Department of Materials Science and Engineering	ATLANTA, GA
	<i>Do Me a Solid: Materials Modeling to Fight Climate Change</i> Carnegie Mellon University Department of Civil and Environmental Engineering	PITTSBURGH, PA
2020	<i>High-Fidelity Accelerated Design of Electrochemical Systems</i> Materials Science & Technology Conference	ONLINE
	<i>Graph Convolutional Networks for Atomic Structures</i> Cambridge Machine Learning Discussion Group	CAMBRIDGE, UK (VIRTUAL)
	<i>Marcus-Hush-Chidsey Kinetics at Solid Surfaces</i> Battery Modeling Webinar Series	ONLINE
	<i>Accelerating Energy Materials Discovery with Computation</i> Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)	NUREMBERG, GERMANY (VIRTUAL)
	<i>Accelerating Energy Materials Discovery with Computation</i> Carnegie Mellon Department of Materials Science and Engineering	PITTSBURGH, PA (VIRTUAL)
2019	<i>Bayesim Workshop</i> Helmholtz Institute for Renewable Energy	NUREMBERG, GERMANY (VIRTUAL)
	<i>Semiconductor Parameter Extraction (and more!) with Bayesian Inference</i> MIT Society of Industrial and Applied Mathematics	CAMBRIDGE, MA
	CONTRIBUTED TALKS	
2023	<i>Modeling Electrochemical Reaction Rates at Fluid-Solid Interfaces</i> MRS Fall Meeting	BOSTON, MA
	<i>Teaching Introductory Materials Science with Pluto Demos</i> JuliaCon	CAMBRIDGE, MA
2022	<i>Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation</i> American Physical Society March Meeting	CHICAGO, IL
2021	<i>Introducing Chemellia: Machine Learning, with Atoms</i> JuliaCon	ONLINE
	<i>Building a Chemistry and Materials Science Ecosystem in Julia</i> JuliaCon (Birds of a Feather discussion leader)	ONLINE
2018	<i>Computational Screening for Defect-Tolerant Semiconductors</i> Gordon Research Seminar on Defects in Semiconductors	NEW LONDON, NH

	<i>Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors</i> Blue Waters Research Symposium	SUNRIVER, OR
2017	<i>Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials</i> Materials Research Society Fall Meeting and Exhibit	BOSTON, MA
2013	<i>Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications</i> Yale Physics Department	NEW HAVEN, CT
2012	<i>Improving Active Layer Performance of Hybrid Photovoltaics by Nano Imprinting with Bulk Metallic Glass</i> Yale Physics Department	NEW HAVEN, CT
	POSTER PRESENTATIONS	
2022	<i>Differentiable Modeling of Electrochemical Reaction Rates</i> Gordon Research Seminar/Conference: Batteries	VENTURA, CA
2020	<i>High-fidelity Accelerated Design of High-performance Electrochemical Systems</i> NeurIPS Climate Change and AI Workshop	ONLINE
2019	<i>Measuring Real-World Quantities from Computer Simulation with Bayesian Inference</i> MIT de Florez Award Competition	CAMBRIDGE, MA
	<i>Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods</i> MIT CCE Symposium	CAMBRIDGE, MA
2018	<i>Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods</i> MIT Materials Day	CAMBRIDGE, MA
	<i>Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors</i> Gordon Research Seminar on Defects in Semiconductors	NEW LONDON, NH
	<i>Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors</i> Blue Waters Research Symposium	SUNRIVER, OR
	<i>Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods</i> World Conference on Photovoltaic Energy Conversion	WAIKOLOA, HI
	<i>Design Principles for Defect-Tolerant Photovoltaic Absorbers</i> MIT de Florez Award Competition	CAMBRIDGE, MA
2016	<i>Quantitative Metrics for Defect Tolerance in Semiconductors</i> Materials Research Society Fall Meeting and Exhibit	BOSTON, MA
	<i>Photovoltaics R&amp;D: Thin Film Materials</i> MIT Energy Night	CAMBRIDGE, MA
	<i>Bayes-Sun Inference: Next-Generation Photovoltaics through Advanced Probabilistic Modeling</i> MIT de Florez Award Competition	CAMBRIDGE, MA
	<i>Statistical Inference of Materials Properties from Solar Cell Measurements</i> Beyond 2016: MIT's Frontiers of the Future Symposium	CAMBRIDGE, MA
2015	<i>Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbers</i> MRS Fall Meeting and Exhibit	BOSTON, MA
	<i>Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials</i> MIT Materials Day	CAMBRIDGE, MA

*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 Quantum Dots*

ITHACA, NY

Northeast Conference for Undergraduate Women in Physics

2012

*Raman Spectroscopy of Silicon Quantum Dots*

GOLDEN, CO

REMRSEC REU Poster Session

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## SERVICE TO THE SCIENTIFIC COMMUNITY

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### 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 &amp; Environmental Science

### CONFERENCE SERVICE

May 2023 **Technical Presentation Judge** CMU MSE GRADUATE SYMPOSIUM2023 – 2024 **Poster Session Judge** CMU ENERGY WEEKMarch 2022 **Session Chair** SCIENTIFIC MACHINE LEARNING WEBINAR SERIESMarch 2022 **Session Chair**, B67: Advanced Approaches in Modeling and Simulation of Defects APS MARCH MEETINGJuly 2021 **Session Chair, Volunteer** JULIACON2021 – present **Reviewer** JULIACON2019 – 2020 **Organizer** PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS2019 **Reviewer** NEURIPS ML4PS WORKSHOPOctober 2019 **Poster Session Judge** PITT SCIENCE20192015 **Organizer** SOLAR ENERGY TECHNOLOGY & INNOVATION IN MEXICO WORKSHOPJanuary 2015 **Panelist** NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS2011 – 2012 **Organizer** NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS

### LEADERSHIP AND UNIVERSITY SERVICE

2023 – present **Member**, Undergraduate Education Committee CMU MSE DEPARTMENT2023 – present **Member**, Open Science Advisory Board CMU LIBRARIESOctober 2023 **Panelist, Mentor** CMU MSE RISING STARS WORKSHOPApril 2023 **Design Judge**, Buggy Design Competition CMU SPRING CARNIVAL2022 – present **Working Group Chair**, Notebooks Now! Initiative AMERICAN GEOPHYSICAL UNION2018 – 2019 **Member**, Graduate Student Advisory Group for Engineering MIT SCHOOL OF ENGINEERING2018 – 2019 **Co-President**, Womxn of Materials Science MIT DMSE2017 **Mentor**, Solar Spring Break (service trip) MIT ENERGY INITIATIVE2016 – 2019 **Member**, Energy Education Task Force MIT ENERGY INITIATIVE2016 – 2019 **Member**, Solar Test Bed Steering Committee MIT OFFICE OF SUSTAINABILITY2015 – 2017 **Co-Leader**, Solar/Grid Community MIT ENERGY CLUB

2012 – 2013	<b>Co-Leader</b> , Project Bright	YALE OFFICE OF SUSTAINABILITY
2012	<b>Co-President</b> , Society of Physics Students	YALE PHYSICS DEPARTMENT
OUTREACH AND OTHER SERVICE		
2022 – present	<b>Mentor</b>	PRISON MATHEMATICS PROJECT
May 2022	<b>Guest Speaker</b>	JULIA GENDER INCLUSIVE
2021 – present	<b>Volunteer</b>	SKYPE A SCIENTIST
2021 – 2022	<b>Grand Award Judge</b> , Materials Science Division	REGENERON ISEF
Summer 2021	<b>GSoC Mentor</b> , Julia Language (Chemellia)	GOOGLE SUMMER OF CODE
March 2014	<b>Demonstrator</b>	CAMBRIDGE HANDS-ON SCIENCE (CHAOS)

## OTHER SKILLS AND ACTIVITIES

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### FOREIGN LANGUAGES

2003 – present	<b>Spanish</b> , proficient
2010 – present	<b>Hebrew</b> , intermediate
2020 – present	<b>Mandarin</b> , 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	<b>Finisher</b> , Ironman Maryland, Ironman 70.3 Musselman, and Pumpkinman Half Iron triathlons
2018 – 2019	<b>Treasurer</b> , MIT Triathlon Team
2014, 2018	<b>Finisher</b> , Stockholm and Marine Corps Marathons
2013 – 2014	<b>Rowing</b> , Churchill College Boat Club (1st Women's VIII in May Bumps 2014)
2009 – 2012	<b>Member</b> (2009 – 2012), <b>Treasurer</b> (2010 – 2011), Yale Bulldog Cycling Team