

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 <b>Guest Lecturer</b> 27-537/27-737: Data Analytics for Materials Science 24-786: Bayesian Machine Learning	CARNEGIE MELLON UNIVERSITY
2022	<b>Guest Lecturer</b> 27-100: Engineering the Materials of the Future 12-623/24-623: Molecular Simulation of Materials	CARNEGIE MELLON UNIVERSITY
2021	<b>Guest Lecturer</b> 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	CARNEGIE MELLON UNIVERSITY
2020	<b>Guest Lecturer</b> 12-623/24-623: Molecular Simulation of Materials 24-786: Bayesian Machine Learning (2 lectures)	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. <b>Graduate Student Teaching Award</b> , School of Engineering	MASSACHUSETTS INSTITUTE OF TECHNOLOGY 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

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HONORS

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2023	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

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RESEARCH SOFTWARE DEVELOPMENT

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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>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 – 2019	<b>Developer</b> , Bayesim Python package for Bayesian parameter estimation from experimental data using high-throughput simulation	<a href="#">GITHUB LINK</a>

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PUBLICATIONS

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

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

2023	<i>It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box</i>	DAVOS, SWITZERLAND
	Platform for Advanced Scientific Computing (PASC) Conference	
	<i>It's All About That Bayes: Data-Driven Insights into Energy Devices without the Black Box</i>	LAS VEGAS, NV
	American Physical Society March Meeting	
	<i>Point Defects in Photovoltaics: From Materials to Devices</i>	EVANSTON, IL
	Snyder Group Meeting, Northwestern University	
2022	<i>Science Stories with Julia</i>	PITTSBURGH, PA (VIRTUAL)
	Jordan Group Meeting, University of Pittsburgh	
	<i>Building a Materials Computation Ecosystem in Julia</i>	OTTAWA, CA (VIRTUAL)
	Institute of Data Science, Carleton University	
	<i>Design of Defect-Tolerant Materials for Photovoltaic Applications</i>	CHICAGO, IL
	American Physical Society March Meeting	
	<i>Building a Materials Computation Ecosystem in Julia</i>	CAMBRIDGE, MA (VIRTUAL)
	MIT CESMIX seminar	
	<i>Accelerating Energy Materials Discovery with Computation</i>	BOSTON, MA (VIRTUAL)
	Boston University Materials Science seminar	
2021	<i>Accelerating Energy Materials Discovery with Computation</i>	ATLANTA, GA
	Georgia Institute of Technology Department of Materials Science and Engineering	
	<i>Do Me a Solid: Materials Modeling to Fight Climate Change</i>	PITTSBURGH, PA
	Carnegie Mellon University Department of Civil and Environmental Engineering	

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)
	<i>Accelerating Energy Materials Discovery with Computation</i> University of Illinois at Urbana-Champaign Department of Electrical & Computer Engineering	URBANA, IL
2019	<i>Bayesim Workshop</i> Helmholtz Institute for Renewable Energy	NUREMBERG, GERMANY (VIRTUAL)
2018	<i>Semiconductor Parameter Extraction (and more!) with Bayesian Inference</i> MIT Society of Industrial and Applied Mathematics	CAMBRIDGE, MA
	CONTRIBUTED TALKS	
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>	CAMBRIDGE, MA
	MIT Materials Day	
	<i>Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors</i>	NEW LONDON, NH
	Gordon Research Seminar on Defects in Semiconductors	
	<i>Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors</i>	SUNRIVER, OR
2016	Blue Waters Research Symposium	
	<i>Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods</i>	WAIKOLOA, HI
	World Conference on Photovoltaic Energy Conversion	
	<i>Design Principles for Defect-Tolerant Photovoltaic Absorbers</i>	CAMBRIDGE, MA
	MIT de Florez Award Competition	
2015	<i>Quantitative Metrics for Defect Tolerance in Semiconductors</i>	BOSTON, MA
	Materials Research Society Fall Meeting and Exhibit	
	<i>Photovoltaics R&amp;D: Thin Film Materials</i>	CAMBRIDGE, MA
	MIT Energy Night	
	<i>Bayes-Sun Inference: Next-Generation Photovoltaics through Advanced Probabilistic Modeling</i>	CAMBRIDGE, MA
2013	MIT de Florez Award Competition	
	<i>Statistical Inference of Materials Properties from Solar Cell Measurements</i>	CAMBRIDGE, MA
	Beyond 2016: MIT's Frontiers of the Future Symposium	
	<i>Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbers</i>	BOSTON, MA
	MRS Fall Meeting and Exhibit	
2012	<i>Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials</i>	CAMBRIDGE, MA
	MIT Materials Day	
	<i>Solar Energy Technology &amp; Innovation in Mexico</i>	CAMBRIDGE, MA
	MIT Energy Initiative Solar Day	
	<i>Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials</i>	GOLDEN, CO
2021	NREL HOPE Workshop	
	<i>Raman Spectroscopy of Silicon Quantum Dots</i>	ITHACA, NY
2020	Northeast Conference for Undergraduate Women in Physics	
	<i>Raman Spectroscopy of Silicon Quantum Dots</i>	GOLDEN, CO
2019	REMRSEC REU Poster Session	

## SERVICE TO THE SCIENTIFIC COMMUNITY

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### JOURNAL EDITING

2021 – present Journal of Open-Source Software

### JOURNAL REVIEWING

2022 – present Computer Physics Communications, APL Machine Learning  
 Journal of Physical Chemistry, Chemistry of Materials, Journal of Physical Chemistry Letters, PR Materials,  
 2021 – present 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

March 2022	<b>Session Chair</b>	SCIENTIFIC MACHINE LEARNING WEBINAR SERIES
March 2022	<b>Session Chair</b> , B67: Advanced Approaches in Modeling and Simulation of Defects	APS MARCH MEETING
July 2021	<b>Session Chair, Volunteer</b>	JULIACON
2021 – present	<b>Reviewer</b>	JULIACON
2019 – 2020	<b>Organizer</b>	PITTSBURGH CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS
2019	<b>Reviewer</b>	NEURIPS ML4PS WORKSHOP
October 2019	<b>Poster Session Judge</b>	PITT SCIENCE2019
2015	<b>Organizer</b>	SOLAR ENERGY TECHNOLOGY & INNOVATION IN MEXICO WORKSHOP
January 2015	<b>Panelist</b>	NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS
2011 – 2012	<b>Organizer</b>	NORTHEAST CONFERENCE FOR UNDERGRADUATE WOMEN IN PHYSICS

## LEADERSHIP/OUTREACH

May 2023	<b>Technical Presentation Judge</b>	CMU MSE GRADUATE SYMPOSIUM
March 2023	<b>Poster Session Judge</b>	CMU ENERGY WEEK
2022 – present	<b>Working Group Chair</b>	NOTEBOOKS NOW! INITIATIVE
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
2018 – 2019	<b>Member</b> , Advisor-Advisee Relations Subcommittee	MIT GRAD STUDENT ADVISORY GROUP FOR ENGINEERING
2018 – 2019	<b>Co-President</b>	MIT WOMEN OF MATERIALS SCIENCE
2017	<b>Mentor</b> , Solar Spring Break (service trip)	MIT ENERGY INITIATIVE
2016 – 2019	<b>Member</b> , Energy Education Task Force	MIT ENERGY INITIATIVE
2016 – 2019	<b>Member</b> , Solar Test Bed Steering Committee	MIT OFFICE OF SUSTAINABILITY
2015 – 2017	<b>Co-Leader</b> , Solar/Grid Community	MIT ENERGY CLUB
March 2014	<b>Demonstrator</b>	CAMBRIDGE HANDS-ON SCIENCE (CHAOS)
2012 – 2013	<b>Co-Leader</b> , Project Bright	YALE OFFICE OF SUSTAINABILITY
2012	<b>Co-President</b> , Society of Physics Students	YALE PHYSICS DEPARTMENT

## OTHER SKILLS AND ACTIVITIES

## 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

2021	<b>Finisher</b> , Ironman Maryland and Ironman 70.3 Musselman triathlons
2019	<b>Finisher</b> , Pumpkinman Half Iron Triathlon
2018 – 2019	<b>Treasurer</b> , MIT Triathlon Team
2014, 2018	<b>Finisher</b> , Stockholm and Marine Corps Marathons
2013 – 2014	<b>Rower</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