

EDUCATION

2014 – 2019	Ph.D. 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	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 Venkat Viswanathan	CARNEGIE MELLON UNIVERSITY
2014 – 2019	PhD student , Materials Science and Engineering Advised by Tonio Buonassisi (Mechanical Engineering) (committee members V. Stevanović, B. Yildiz, J. Grossman)	MASSACHUSETTS INSTITUTE OF TECHNOLOGY
2016 – 2018	Visiting student , Solar Energy Research Facility Summer stays advised by Vladan Stevanović	NATIONAL RENEWABLE ENERGY LABORATORY
2013 – 2014	MPhil student , Materials Science & Metallurgy Supervised by Stoyan Smoukov, advised by Dame Athene Donald (Physics)	UNIVERSITY OF CAMBRIDGE
2012 – 2013	Undergraduate researcher , Physics (senior thesis) Advised by Minjoo Larry Lee (Electrical Engineering)	YALE UNIVERSITY
Summer 2012	REU Student , Renewable Energy MRSEC Advised by Thomas Furtak (Physics)	COLORADO SCHOOL OF MINES
2012	Undergraduate researcher , Physics Advised by Chinedum Osuji (Chemical Engineering)	YALE UNIVERSITY
Summer 2011	Undergraduate researcher , Earth and Planetary Sciences Advised by Ilan Koren	WEIZMANN INSTITUTE OF SCIENCE
Summer 2008	High school summer researcher , Laboratory for Laser Energetics Advised by R. Stephen Craxton and Mark Wittman	UNIVERSITY OF ROCHESTER

TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION

2023	Instructor , 27-100: Engineering the Materials of the Future	CARNEGIE MELLON UNIVERSITY
2021	Guest Lecturer 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	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 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 3.23: Electronic, Optical, and Magnetic Properties of Materials	MASSACHUSETTS INSTITUTE OF TECHNOLOGY
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*, in press.
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**[†], 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 A₃Sb₂I₉ 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 (BiI₃) for photovoltaic applications." *J. Phys. Chem. Lett.* **6**, 4297-4302 (2015)

PRESENTATIONS

INVITED TALKS

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
	APS 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 (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	
2020	High-Fidelity Accelerated Design of Electrochemical Systems	ONLINE
	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

2018 *Semiconductor Parameter Extraction (and more!) with Bayesian Inference* CAMBRIDGE, MA
MIT Society of Industrial and Applied Mathematics

CONTRIBUTED TALKS

2022 *Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation* CHICAGO, IL
American Physical Society March Meeting

2021 *Introducing Chemellia: Machine Learning, with Atoms* ONLINE
JuliaCon

Building a Chemistry and Materials Science Ecosystem in Julia ONLINE
JuliaCon (Birds of a Feather discussion leader)

2018 *Computational Screening for Defect-Tolerant 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

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

2013 *Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications* NEW HAVEN, CT
Yale Physics Department

2012 *Improving Active Layer Performance of Hybrid Photovoltaics by Nano Imprinting with Bulk Metallic Glass* NEW HAVEN, CT
Yale Physics Department

POSTER PRESENTATIONS

2022 *Differentiable Modeling of Electrochemical Reaction Rates* VENTURA, CA
Gordon Research Seminar/Conference: Batteries

2020 *High-fidelity Accelerated Design of High-performance Electrochemical Systems* ONLINE
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

2018 *Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods* CAMBRIDGE, MA
MIT Materials Day

Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors NEW LONDON, NH
Gordon Research Seminar on Defects in Semiconductors

	<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&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
	<i>Solar Energy Technology & Innovation in Mexico</i> MIT Energy Initiative Solar Day	CAMBRIDGE, MA
	<i>Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials</i> NREL HOPE Workshop	GOLDEN, CO
2013	<i>Raman Spectroscopy of Silicon Quantum Dots</i> Northeast Conference for Undergraduate Women in Physics	ITHACA, NY
2012	<i>Raman Spectroscopy of Silicon Quantum Dots</i> REMRSEC REU Poster Session	GOLDEN, CO

SERVICE TO THE SCIENTIFIC COMMUNITY

JOURNAL EDITING

2021 – present	Journal of Open-Source Software
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JOURNAL REVIEWING

2022 – present	Computer Physics Communications
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

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
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/OUTREACH

2022 – present	Working Group Chair	NOTEBOOKS NOW! INITIATIVE
2022 – present	Mentor	PRISON MATHEMATICS PROJECT
May 2022	Guest Speaker	JULIA GENDER INCLUSIVE
2021 – present	Volunteer	SKYPE A SCIENTIST
2021 – present	Grand Award Judge , Materials Science Division	REGENERON ISEF
Summer 2021	GSoC Mentor , Julia Language (Chemellia)	GOOGLE SUMMER OF CODE
2018 – 2019	Member , Advisor-Advisee Relations Subcommittee	MIT GRAD STUDENT ADVISORY GROUP FOR ENGINEERING
2018 – 2019	Co-President	MIT WOMEN OF MATERIALS SCIENCE
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
March 2014	Demonstrator	CAMBRIDGE HANDS-ON SCIENCE (CHAOS)
2012 – 2013	Co-Leader , Project Bright	YALE OFFICE OF SUSTAINABILITY
2012	Co-President , Society of Physics Students	YALE PHYSICS DEPARTMENT

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

2021	Finisher , Ironman Maryland and Ironman 70.3 Musselman triathlons
2019	Finisher , Pumpkinman Half Iron Triathlon
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