curriculum vitæ of

Rachel C. Kurchin

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

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EDUCATION

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	CARNEGIE MELLON UNIVERSITY

Advised by Venkat Viswanathan, supported by MFI and MolSSI fellowships

2014 – 2019	**PhD student**, Materials Science and Engineering	MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Advised by Tonio Buonassisi (Mechanical Engineering) (committee members V. Stevanović, B. Yildiz, J. Grossman)

2016 – 2018	**Visiting student**, Solar Energy Research Facility	NATIONAL RENEWABLE ENERGY LABORATORY

Summer stays advised by Vladan Stevanović

2013 – 2014	**MPhil student**, Materials Science & Metallurgy	UNIVERSITY OF CAMBRIDGE

Supervised by Stoyan Smoukov, advised by Dame Athene Donald (Physics)

2012 – 2013	**Undergraduate researcher**, Physics (senior thesis)	YALE UNIVERSITY

Advised by Minjoo Larry Lee (Electrical Engineering)

Summer 2012	**REU Student**, Renewable Energy MRSEC	COLORADO SCHOOL OF MINES

Advised by Thomas Furtak (Physics)

2012	**Undergraduate researcher**, Physics	YALE UNIVERSITY

Advised by Chinedum Osuji (Chemical Engineeing)

Summer 2011	**Undergraduate researcher**, Earth and Planetary Sciences	WEIZMANN INSISTUTE OF SCIENCE

Advised by Ilan Koren

Summer 2008	**High school summer researcher**, Laboratory for Laser Energetics	UNIVERSITY OF ROCHESTER

Advised by R. Stephen Craxton and Mark Wittman

TEACHING EXPERIENCE, PREPARATION, AND RECOGNITION

2023	**Instructor**, 27-100: Engineering the Materials of the Future	CARNEGIE MELLON UNIVERSITY
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**	CARNEGIE MELLON UNIVERSITY

12-623/24-623: Molecular Simulation of Materials
24-786: Bayesian Machine Learning (2 lectures)

	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**	MASSACHUSETTS INSTITUTE OF TECHNOLOGY

3.23: Electronic, Optical, and Magnetic Properties of Materials

2011 – 2013	**Science and Quantitative Reasoning Tutor**, Dean's Office	YALE UNIVERSITY

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 $A_3Sb_2I_9$ 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_3) for photovoltaic applications." *J. Phys. Chem. Lett. 6, 4297-4302 (2015)*

Research Software Development

2021 – present   **Co-Developer**, AtomsBase   Github link

Julia interface for representing atomic structures and enabling interoperability between codes, 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, comprising a number of packages for featurization, modeling, etc.

2017 – 2019	**Developer**, Bayesim	GITHUB LINK

Python package for Bayesian parameter estimation from experimental data using high-throughput simulation

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

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

2021	*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	
	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	
2016	*Quantitative Metrics for Defect Tolerance in Semiconductors*	BOSTON, MA
	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	
2015	*Improving the Accuracy of Novel Materials Screening: Growing Defect-Tolerant Photovoltaic Absorbers*	BOSTON, MA
	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	
2012	*Raman Spectroscopy of Silicon Quntum Dots*	GOLDEN, CO
	REMRSEC REU Poster Session	

SERVICE TO THE SCIENTIFIC COMMUNITY

JOURNAL EDITING

2021 – present	Journal of Open-Source Software

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

May 2022	**Guest Speaker**	Julia Gender Inclusive
2021 – present	**Grand Award Judge**, Materials Science Division	Regeneron ISEF
Sumer 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