

curriculum vitae of  
**Rachel C. Kurchin**

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

 [rkurchin.github.io](https://github.com/rkurchin)    [rkurchin@cmu.edu](mailto:rkurchin@cmu.edu)    [google scholar](https://scholar.google.com/citations?user=...)    [github](https://github.com/rkurchin)

## 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	MATERIALS RESEARCH SOCIETY FALL MEETING
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
	Graduate Student Teaching Award	MIT DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING
	Graduate Student Teaching Award	MIT SCHOOL OF ENGINEERING
	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
2013	Gates Cambridge Scholarship	CAMBRIDGE GATES TRUST
	Howard L. Schulz Prize	YALE PHYSICS DEPARTMENT

## RESEARCH SOFTWARE DEVELOPMENT

2021 – present	<b>Co-Developer</b> , AtomsBase	<a href="#">GITHUB LINK</a>
2020 – present	<b>Lead Developer</b> , ElectrochemicalKinetics	<a href="#">GITHUB LINK</a>
2020 – present	<b>Lead Developer</b> , Chemellia	<a href="#">GITHUB LINK</a>
2017 – present	<b>Lead Developer</b> , Bayesim	<a href="#">GITHUB LINK</a>

## PUBLICATIONS

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

21. M. Babar, Z. Zhu, **R. C. Kurchin**, E. Kaxiras, and V. Viswanathan. “Twisto-Electrochemical Activity Volcanoes in Trilayer Graphene” *J. Am. Chem. Soc.* (2024)
20. X. Wang, J. Musielewicz, R. Tran, S. K. Ethirajan, X. Fu, H. Mera, J. R. Kitchin, **R. C. Kurchin**, and Z. W. Ulissi. “Generalization of graph-based active learning relaxation strategies across materials” *Mach. learn.: sci. technol.* (2024)
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†, **R. C. Kurchin**†, 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 interfaces.” *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)

## SELECTED INVITED TALKS

2024	<i>Materials Modeling: Bonding across Atoms, Code, and People</i> JuliaCon ( <b>keynote</b> )	EINDHOVEN, THE NETHERLANDS
	<i>Using Computation to Accelerate Materials Engineering, from the Atomistic to Device Scale</i> IEEE Photovoltaic Specialists Conference ( <b>plenary</b> )	SEATTLE, WA
	<i>Learning from Data and Distributions to Accelerate Engineering of Energy Materials and Devices</i> MRS Spring Meeting	SEATTLE, WA
2023	<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
2022	<i>Design of Defect-Tolerant Materials for Photovoltaic Applications</i> American Physical Society March Meeting	CHICAGO, IL
2021	<i>Accelerating Energy Materials Discovery with Computation</i> Georgia Institute of Technology Department of Materials Science and Engineering	ATLANTA, GA
	<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