# Rachel C. Kurchin

Carnegie Mellon University Pittsburgh, PA		rkurchin@cmu.edu rkurchin.github.io	
EDUCATION	ON		
2019	Massachusetts Institute of Technology Cambridge, MA, USA Ph.D., Materials Science and Engineering, GPA 4.6/5.0		
2014	University of Cambridge Cambridgeshire, UK MPhil, Materials Science & Metallurgy (research-based)		
2013	Yale University New Haven, CT, USA B.S., Physics (Intensive), with distinction (magna cum laude, GPA 3.9/4.0)		
RESEARC	H POSITIONS		
2019 – pres.	Carnegie Mellon University Mechanical Engineering, Materials S MFI ('19-'20), MolSSI ('21) Postdoctoral Fellow with Venkat Viswana		
2014 - 2019	Massachusetts Institute of Technology Mechanical Engineering Ph.D. student with Tonio Buonassisi (committee: V. Stevanović, J. Grossman, B. Yildiz)		
2016 - 2017	National Renewable Energy Laboratory Solar Energy Research Facility Summer Visiting Graduate Student with Vladan Stevanović		
2013 - 2014	University of Cambridge Materials Science & Metallurgy Master's Student with Stoyan Smoukov, advised by Dame Athene Donald		
2012 - 2013	Yale University Electrical Engineering Undergraduate researcher (senior thesis) with Minjoo Larry Lee		
2012	Colorado School of Mines Physics REMRSEC REU Student with Thomas Furtak		
2012	Yale University Chemical Engineering Undergraduate researcher with Chinedum Osuji		
2011	Weizmann Institute of Science Earth and Planetary Sciences Undergraduate summer researcher with Ilan Koren		
2008	University of Rochester Laboratory for Laser Energetics High school summer researcher with R. Stephen Craxton		
TEACHING	G EXPERIENCE, PREPARATION, AND RECOGNITION		
2021	Guest lecturer CMU Courses 12-623/24-623: Molecular Simulation	n of Materials	
	24-643/27-700: Energy Storage Mate	erials and Systems	
	12-216: Introduction to Research Ski	lls in CEE	
2020	Guest lecturer CMU Courses 12-623/24-623: Molecular Simulation	n of Materials	
	24-786: Bayesian Machine Learning	(2 lectures)	
	Future Faculty Program CMU Eberly Center for Teaching Excelle	ence	
2019	Graduate Student Teaching Award MIT Department of Material	s Science and Engineering	
	Graduate Student Teaching Award MIT School of Engineering		

2018 **Teaching Assistant** MIT Dept. of Materials Science and Engineering 3.23: Electronic, Optical, and Magnetic Properties of Materials

2011 - 2013 Science and Quantitative Reasoning Tutor Yale University Dean's Office

### FELLOWSHIPS AND AWARDS

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 Initiative
	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 Dept. of Mechanical Engineering
2014	GRFP Honorable Mention National Science Foundation
2013	Gates Cambridge Scholarship Cambridge Gates Trust
	Howard L. Schultz Prize Yale Physics Department
2012	Mellon Grant Pierson College at Yale University
	REMRSEC REU Technical Achievement Award Colorado School of Mines Renewable Energy Materials Research Science and Engineering Center
2009	Robert C. Byrd Honors Scholarship US Department of Education
	Intel STS Semifinalist Intel Science Talent Search

#### PUBLICATIONS (Google Scholar)

- 2021 [16] A. Mistry, A. Verma, S. Sripad, R. Ciez, V. Sulzer, F. Brosa Planella, R. Timms, Y. Zhang, R. Kurchin, et al. "A minimal information set to enable verifiable theoretical battery research."

  ACS Energy Letters 3831–3835 (2021)
- 2020 [15] **R. Kurchin**, V. Viswanathan. "Marcus-Hush-Chidsey kinetics at electrode-electrolyte interfaces." *The Journal of Chemical Physics* 153, 134706 (2020)
  - [14] R. C. Kurchin, J. R. Poindexter, V. Vahanissi, et al. "How much physics is in a current-voltage curve? Inferring defect properties from photovoltaic device measurements." *IEEE Journal of Photovoltaics* 10, 1532–1537 (2020)
- 2019 [13] **R. C. Kurchin**, G. Romano, T. Buonassisi. "Bayesim: a tool for adaptive grid model fitting with Bayesian inference." *Computer Physics Communications* 239, 161–165 (2019)
- 2018 [12] **R. C. Kurchin**, P. Gorai, T. Buonassisi, V. Stevanović. "Structural and chemical features giving rise to defect tolerance of binary semiconductors." *Chemistry of Materials* 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." *Chemistry of Materials* 30, 3734–3742 (2018)

- 2017 [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." *Chemistry of Materials* 30, 336–343 (2017)
  - [09] R. Brandt, R. C. Kurchin, V. Steinmann, et al. "Rapid semiconductor device characterization through Bayesian parameter estimation." *Joule* 1, 843–856 (2017)
  - [08] R. Hoye, L. C. Lee, **R. C. Kurchin**, et al. "Strongly enhanced photovoltaic performance and defect physics of air-stable bismuth oxylodide (BiOI)." *Advanced Materials* 29, (2017)
  - [07] R. E. Brandt, J. Poindexter, P. Gorai, R. Kurchin, et al. "Searching for "defect-tolerant" photovoltaic materials: combined theoretical and experimental screening." Chemistry of Materials 29, 4667–4674 (2017)
  - [06] 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)
- 2016 [05] R. Hoye, P. Schulz, L. T. Schelhas, A. M. Holder, K. H. Stone, J. D. Perkins, D. Vigil-Fowler, S. Siol, D. O. Scanlon, A. Zakutayev, A. Walsh, I. C. Smith, B. C. Melot, R. C. Kurchin, et al. "Perovskite-inspired photovoltaics: best practices in materials characterization and calculations." Chemistry of Materials 29, 1964–1988 (2016)
  - [04] D. B. Needleman, J. R. Poindexter, R. C. Kurchin, et al. "Economically sustainable scaling of photovoltaics to meet climate targets." *Energy & Environmental Science* 9, 2122–2129 (2016)
  - [03] A. Gufan, Y. Lehahn, E. Fredj, C. Price, R. C. Kurchin, et al. "Segmentation and tracking of marine cellular clouds observed by geostationary satellites." *International Journal of Remote* Sensing 37, 1055–1068 (2016)
- 2015 [02] R. Hoye, R. E. Brandt, A. Osherov, V. Stevanović, S. D. Stranks, M. Wilson, H. Kim, A. J. Akey, **R. C. Kurchin**, et al. "Methylammonium bismuth iodide as a lead-free, stable hybrid organic-inorganic solar absorber." *Chemistry A European Journal* 22, 2605–2610 (2015)
  - [01] R. E. Brandt, R. C. Kurchin, R. Hoye, et al. "Investigation of bismuth triiodide (BiI<sub>3</sub>) for photovoltaic applications." *The Journal of Physical Chemistry Letters* 6, 4297–4302 (2015)

#### INVITED TALKS

2022 Chemellia: Machine Learning, with Atoms!

Rowley Group Seminar, Ottawa, Canada (virtually)

Design of Defect-Tolerant Materials for Photovoltaic Applications

APS March Meeting, Chicago, IL

Chemellia: Machine Learning, with Atoms!

MIT CESMIX seminar, Cambridge, MA (virtually)

2021 Accelerating Energy Materials Discovery with Computation

Georgia Institute of Technology, Atlanta, GA (virtually)

Do Me a Solid: Materials Modeling to Fight Climate Change

Carnegie Mellon Department of Civil and Environmental Engineering, Pittsburgh, PA

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

Materials Science & Technology Conference, online

 $Graph\ Convolutional\ Networks\ for\ Atomic\ Structures$ 

Seminar Cambridge Machine Learning Discussion Group, Cambridge, UK

Marcus-Hush-Chidsey Kinetics at Solid Surfaces

Battery Modeling Webinar Series, online

Accelerating Energy Materials Discovery with Computation

Friedrich-Alexander-Universitt Erlangen-Nrnberg (FAU), virtually in Nuremberg, Germany

Accelerating Energy Materials Discovery with Computation

Carnegie Mellon University Materials Science and Engineering Department, online

Accelerating Energy Materials Discovery with Computation

UIUC Electrical & Computer Engineering Department, Urbana, IL

2019 Bayesim Workshop

Helmholtz Institute for Renewable Energy, virtually in Nuremberg, Germany

2018 Semiconductor Parameter Extraction (and more!) with Bayesian Inference

MIT Society of Industrial and Applied Mathematics, Cambridge, MA

#### CONTRIBUTED TALKS

2022	Non-equilibrium Electrochemical Phase Diagrams with Automatic Differentiation APS March Meeting, Chicago, IL
2021	Introducing Chemellia: Machine Learning, with Atoms JuliaCon, online
	Building a Chemistry and Materials Science Ecosystem in Julia JuliaCon, online
2018	Computational Screening for Defect-Tolerant Semiconductors Gordon Research Seminar on Defects in Semiconductors, New London, NH
	Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors Blue Waters Research Symposium, Sunriver, OR
2017	Toward Quantitative Metrics to Screen for Defect Tolerance in Novel Semiconducting Materials Materials Research Society Fall Meeting and Exhibit, Boston, MA
2013	Cross-Sectional EBIC Characterization of III-V Semiconductors for Photovoltaic Applications Yale Physics Department, New Haven, CT
2012	Improving Active Layer Performance of Hybrid Photovoltaics by Nano Imprinting with Bulk Metallic Glass

## POSTER PRESENTATIONS

Yale Physics Department, New Haven, CT

2020	High-fidelity Accelerated Design of High-performance Electrochemical Systems NeurIPS 2020 Climate Change and AI Workshop, online
2019	Measuring Real-World Quantities from Computer Simulation with Bayesian Inference MIT de Florez Award Competition, Cambridge, MA
	Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods MIT CCE Symposium, Cambridge, MA
2018	Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods MIT Materials Day, Cambridge, MA
	Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors Blue Waters Research Symposium, Sunriver, OR
	Semiconductor Parameter Extraction via Current-Voltage Characterization and Bayesian Inference Methods World Conference on Photovoltaic Energy Conversion, Waikoloa, HI

Design Principles for Defect-Tolerant Photovoltaic Absorbers

MIT de Florez Award Competition, Cambridge, MA 2016 Quantitative Metrics for Defect Tolerance in Semiconductors Materials Research Society Fall Meeting and Exhibit, Boston, MA Photovoltaics R&D: Thin Film Materials MIT Energy Night, Cambridge, MA Bayes-Sun Inference: Next-Generation Photovoltaics through Advanced Probabilistic Modeling MIT de Florez Award Competition, Cambridge, MA Statistical Inference of Materials Properties from Solar Cell Measurements Beyond 2016: MIT's Frontiers of the Future Symposium, Cambridge, MA 2015 Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials MIT Materials Day, Cambridge, MA Solar Energy Technology & Innovation in Mexico MIT Energy Initiative Solar Day, Cambridge, MA Toward Algorithmic Screening of Novel, Defect-Tolerant Solar Materials NREL HOPE workshop, Golden, CO 2013 Raman Spectroscopy of Silicon Quntum Dots

#### SERVICE

2012

#### Journal Editor

since 2021 **Journal of Open-Source Software** Open Journals

Raman Spectroscopy of Silicon Quntum Dots REMRSEC REU Poster Session, Golden, CO

## Journal Reviewer

since 2021 Journal of Physical Chemistry Americal Chemical Society

Chemistry of Materials Americal Chemical Society

Journal of Physical Chemistry Letters American Chemical Society

Northeast Conference for Undergraduate Women in Physics, Ithaca, NY

PR Materials Physical Review Journals

JuliaCon

Computational Materials Science Elsevier

Journal of Photovoltaics IEEE

 ${\bf Nature} \ {\bf Computational} \ {\bf Science} \ {\it Springer} \ {\it Nature}$ 

since 2020 NPJ Computational Materials Springer Nature

since 2019 Applied Energy Materials American Chemical Society

since 2017 Energy & Environmental Science Royal Society of Chemistry

<u>Conferences</u>

March 2022 Session Chair APS March Meeting

B67: Advanced Approaches in Modeling and Simulation of Defects

K67: Quantum Emitters and Spin Devices

July 2021 Session Chair, Volunteer JuliaCon

2019 – 2020 Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics

2019 Reviewer NeurIPS ML4PS Workshop

2011 - 2012	Conference Organizer Northeast Conference for Undergraduate Women in Physics	
Leadership/Outreach		
2021-present	Grand Award Judge Regeneron ISEF	
2018 - 2019	Graduate Student Advisory Group for Engineering MIT School of Engineering	
2018 - 2019	Co-President, Women of Materials Science MIT Department of Materials Science	
Spring 2017	Graduate Student Mentor, Solar Spring Break MIT Energy Initiative	
2016 - 2019	Energy Education Task Force MIT Energy Initiative	
2016 - 2019	Solar Test Bed Steering Committee MIT Office of Sustainability	
2015 - 2017	Solar/Grid Community Co-Leader MIT Energy Club	
March 2014	Science Demonstrator Cambridge Hands-On Science	
2012 - 2013	Project Bright Co-Leader Yale University	
2012	SPS Co-President Yale Society of Physics Students	

Conference Organizer Solar Energy Technology & Innovation in Mexico Workshop

Graduate Student Panelist Northeast Conference for Undergraduate Women in Physics

#### COMPUTATIONAL SKILLS

Simulation	VASP	GPAW	PC1D	SCAPS-1D
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Languages Julia, Python, Matlab, Mathematica, LATEX, bash

HPC Have earned allocations and used systems at national labs, NSF facilities, and universities

Software Git, GitHub, open-source package development and maintenance in Julia and Python incl. CI,

Development docs, issues/PR's, etc.

## OTHER SKILLS AND ACTIVITIES

	Languages

2015

January 2015

Spanish Proficient Hebrew Intermediate Mandarin Beginner

## Music – Violinist

2014 - 2019	MIT Chamber Music Society, MIT Gilbert & Sullivan Players, MIT Musical Theater Guild
2009 - 2013	Jonathan Edwards College Philharmonic, Pit orchestras for the Yale Dramat, Yale Gilbert & Sullivan Society, Opera Theatre of Yale College, and various independent productions
Athletics	
2021	Finish on January Mandaud and January 70.2 Manashary triables

## 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 womens VIII in May Bumps 2014)

2009 – 2012 — Member (2009 – 2012), Manager (2010 – 2011), Yale Bulldog Cycling Team