# Rachel C. Kurchin

Carnegie Mel Pittsburgh, F	lon University A	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 Viswan	
2014 - 2019	Massachusetts Institute of Technology Mechanical Engineering Ph.D. student with Tonio Buonassisi (committee: V. Stevanović, J. C	Grossman, B. Yildiz)
2016 - 2017	National Renewable Energy Laboratory Solar Energy Research Summer Visiting Graduate Student with Vladan Stevanović	Facility
2013 - 2014	University of Cambridge Materials Science & Metallurgy Master's Student with Stoyan Smoukov, advised by Dame Athene Do	onald
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	
	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

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 oxyiodide (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

2021 Role of Defects in Photovoltaic Materials
APS March Meeting, Chicago, IL
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-Universität Erlangen-Nürnberg (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

# CONTRIBUTED TALKS

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 Yale Physics Department, New Haven, CT

2012	Metallic Glass Yale Physics Department, New Haven, CT
POSTEI	R PRESENTATIONS
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 Northeast Conference for Undergraduate Women in Physics, Ithaca, NY
2012	Raman Spectroscopy of Silicon Quntum Dots REMRSEC REU Poster Session, Golden, CO

# REVIEWING/EDITING

Editor	
since $2021$	Journal of Open-Source Software Open Journals
Reviewer	
since 2021	Chemistry of Materials Americal Chemical Society
	Journal of Physical Chemistry Letters American Chemical Society
	PR Materials Physical Review Journals
	JuliaCon
	Computational Materials Science Elsevier
	Journal of Photovoltaics IEEE
	Nature Computational Science Springer Nature
since $2020$	NPJ Computational Materials Springer Nature
2019	NeurIPS ML4PS Workshop
since 2019	Applied Energy Materials American Chemical Society
since $2017$	Energy & Environmental Science Royal Society of Chemistry
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SERVICE	
SERVICE July 2021	$\textbf{Session Chair, Volunteer} \ \textit{JuliaCon}$
	Session Chair, Volunteer JuliaCon
July 2021	Session Chair, Volunteer JuliaCon
July 2021 2021 – present	Session Chair, Volunteer JuliaCon Grand Award Judge Regeneron ISEF
July 2021 2021 – present 2019 – 2020	Session Chair, Volunteer JuliaCon Grand Award Judge Regeneron ISEF Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics
July 2021 2021 – present 2019 – 2020 2018 – 2019	Session Chair, Volunteer JuliaCon Grand Award Judge Regeneron ISEF Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics Graduate Student Advisory Group for Engineering MIT School of Engineering
July 2021 2021 – present 2019 – 2020 2018 – 2019 2018 – 2019	Session Chair, Volunteer JuliaCon Grand Award Judge Regeneron ISEF Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics Graduate Student Advisory Group for Engineering MIT School of Engineering Co-President, Women of Materials Science MIT Department of Materials Science
July 2021 2021 – present 2019 – 2020 2018 – 2019 2018 – 2019 Spring 2017	Session Chair, Volunteer JuliaCon Grand Award Judge Regeneron ISEF Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics Graduate Student Advisory Group for Engineering MIT School of Engineering Co-President, Women of Materials Science MIT Department of Materials Science Graduate Student Mentor, Solar Spring Break MIT Energy Initiative
July 2021 2021 – present 2019 – 2020 2018 – 2019 2018 – 2019 Spring 2017 2016 – 2019	Session Chair, Volunteer JuliaCon Grand Award Judge Regeneron ISEF Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics Graduate Student Advisory Group for Engineering MIT School of Engineering Co-President, Women of Materials Science MIT Department of Materials Science Graduate Student Mentor, Solar Spring Break MIT Energy Initiative Energy Education Task Force MIT Energy Initiative
July 2021 2021 – present 2019 – 2020 2018 – 2019 2018 – 2019 Spring 2017 2016 – 2019 2016 – 2019	Session Chair, Volunteer JuliaCon Grand Award Judge Regeneron ISEF Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics Graduate Student Advisory Group for Engineering MIT School of Engineering Co-President, Women of Materials Science MIT Department of Materials Science Graduate Student Mentor, Solar Spring Break MIT Energy Initiative Energy Education Task Force MIT Energy Initiative Solar Test Bed Steering Committee MIT Office of Sustainability
July 2021 2021 – present 2019 – 2020 2018 – 2019 2018 – 2019 Spring 2017 2016 – 2019 2016 – 2019 2015	Session Chair, Volunteer JuliaCon Grand Award Judge Regeneron ISEF Conference Organizer Pittsburgh Conference for Undergraduate Women in Physics Graduate Student Advisory Group for Engineering MIT School of Engineering Co-President, Women of Materials Science MIT Department of Materials Science Graduate Student Mentor, Solar Spring Break MIT Energy Initiative Energy Education Task Force MIT Energy Initiative Solar Test Bed Steering Committee MIT Office of Sustainability Conference Organizer Solar Energy Technology & Innovation in Mexico Workshop

2012 – 2013 Project Bright Co-Leader Yale University

2012 SPS Co-President Yale Society of Physics Students

2011 – 2012 Conference Organizer Northeast Conference for Undergraduate Women in Physics

#### COMPUTATIONAL SKILLS

Simulation VASP, GPAW, PC1D, SCAPS-1D

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

# Foreign Languages

Spanish Proficient Hebrew Intermediate

# 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 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), Manager (2010 – 2011), Yale Bulldog Cycling Team